# AN INVERSE EIGENVALUE PROBLEM FOR A ONE-DIMENSIONAL SCHRÖDINGER EQUATION WITH VARYING POTENTIAL AND APPLICATIONS TO COMPUTING RESONANCE ENERGY OF MOLECULES

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Abstract. The regularized analytical continuation method (RAC) proved to be a very powerful method for determination of resonance energies and resonance widths of several atomic and molecular systems including large systems of biological importance. For correct applications of the RAC method the knowledge of the asymptotic behavior of the basic ingredient of the method, the coupling function $\lambda(\kappa)$, is important. In this paper we find the correct asymptotic form of $\lambda(\kappa)$ for broad class of realistic potentials and for nonzero values of the angular momentum. To the best of our knowledge this problem has never been studied before.

## 1. Introduction

Resonances in non-relativistic quantum mechanics are defined as solutions of the Schrödinger equation

$$-\frac{d^2\psi_l(r)}{dr^2} + \frac{l(l+1)}{r^2}\psi_l(r) + U(r)\psi_l(r) = k^2\psi_l(r) \tag{1}$$

$l = 0, 1, 2, ...$ satisfying the Siegert boundary conditions [1]

$$\psi_l(0) = 0, \qquad \frac{\psi_l'(R)}{\psi_l(R)} = ik, \tag{2}$$

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where $R$ is a distance from the origin at which the interaction $U(r) = 0$. It is important to mention that the eigenvalue $k$ enters the boundary condition Eq.(2) and thus the problem to find the eigenvalue $k$ is nonlinear. Generally all the eigenvalues can be divided into three groups [2]:

- Im $k > 0$, Re k = 0, bound states. These states are easily calculated because the solution $\psi_l(r) \in L_2$.
- Im $k < 0$, Re k = 0, virtual states
- Im $k < 0$, Re k $\neq$ 0, resonance states.

Both resonance and virtual states are difficult to calculate because the solution $\psi_l(r)$ at large distances oscillates and exponentially increases.

Recently the so-called method of regularized analytical continuation [3] was proposed and has been successfully applied to a broad range of systems from atomic resonances to resonances formed by collisions of electrons with large molecules [4], [5], [6]. It is well known that the process of analytical continuation represents an ill-posed problem. It is the purpose of this paper to improve the accuracy and stability of the RAC method by studying the analytical features of the so-called coupling function. Rigorous mathematical proof of asymptotic behavior of the coupling function $\lambda(\kappa)$ is provided for a broad class of potentials for nonzero values of the angular momentum $l$.

1.1. **RAC method.** The essence of the RAC method consists in changing the strength of the potential $U(r)$

$$U(r) \to (1+\lambda)U(r) \tag{3}$$

so that the resonance states are analytically continued into the bound state region. In the bound state region we have

$$-\frac{d^2\psi_l(r)}{dr^2} + \frac{l(l+1)}{r^2}\psi_l(r) + (1+\lambda)U(r)\psi_l(r) = -\kappa^2\psi_l(r) \tag{4}$$

where the energy $E$ is negative, $E = k^2 = -\kappa^2, k = i\kappa$ and $\psi_l(r) \in L_2$. The energy $E = -\kappa^2$ depends now also on the strength parameter $\lambda$, i.e. $\kappa = \kappa(\lambda)$ and similarly we can define the inverse function $\lambda = \lambda(\kappa)$. The resonances are then found by solving the equation

$$\lambda(\kappa) = 0. \tag{5}$$

As mentioned above the potential $U(r)$ is assumed to be of short-range (i.e. decaying faster than any negative power of $r$ as $r \to +\infty$). As a typical example we can imagine the potential in the form of the Gaussian potential

$$U(r) = ae^{-br^2}, \qquad a < 0. \tag{6}$$

This potential has been used in nuclear physics as a potential model in the theory of nucleon-nucleon scattering (see e.g. [7]) as well as in quantum chemistry. Several low-energy (small $\kappa$) approximate expression of the function $\lambda(\kappa)$ have been proposed [8], [9], [10] but it seems impossible to compute $\lambda(\kappa)$ exactly.

The lowest RAC approximation, the [2/1] approximation, is

$$\lambda^{[2/1]}(\kappa) = \lambda_0 \frac{\kappa^2 + 2\alpha^2\kappa + \alpha^4 + \beta^2}{\alpha^4 + \beta^2 + 2\alpha^2\kappa}. \tag{7}$$

This function has two complex conjugate zeros

$$\kappa_{1,2} = -\alpha^2 \pm i\beta.$$

or in $k$-space

$$k_{1,2} = \pm\beta - i\alpha^2$$

and obviously describes one pair of resonances with the energy $E = \beta^2 - \alpha^4$ and width $\Gamma = 4\alpha^2\beta$. The parameters $\alpha$ and $\beta$ have direct physical meaning determining the real and imaginary parts of the resonance energy. To get the resonance parameters this function has to be fitted to the input data. The standard way is to minimize the following functional

$$\chi^2 = \sum_{i=1}^{N} \left|\lambda(\kappa_i) - \lambda_i\right|^2. \tag{8}$$

where $N$ is the number of input points $\{\lambda_i\}$ and the corresponding bound state energies $\{E_i = -\kappa_i^2\}$. The function $\lambda(\kappa)$ in the [2/1] approximation, Eq.(7), increases linearly as $\kappa \to \infty$.

If one virtual state is added to the pair of resonances we get a [3/1] PA

$$\lambda^{[3/1]}(\kappa) = \lambda_0 \frac{(\kappa^2 + 2\alpha^2\kappa + \alpha^4 + \beta^2)(1 + \delta^2\kappa)}{\alpha^4 + \beta^2 + \kappa(2\alpha^2 + \delta^2(\alpha^4 + \beta^2))}. \tag{9}$$

In this case we have one additional parameter -$\delta$ to fit. This parameter determines the energy of the virtual state $E_v = -\delta^{-4}$. Now the function $\lambda(\kappa)$ behaves as $\kappa^2$ at large $\kappa$.

The same set of resonance parameters, i.e. $\alpha, \beta, \delta$, is described by the [3/2] approximation

$$\lambda^{[3/2]}(\kappa) = \lambda_0 \frac{(\kappa^2 + 2\alpha^2\kappa + \alpha^4 + \beta^2)(1 + \delta^2\kappa)}{\alpha^4 + \beta^2 + \kappa(2\alpha^2 + \delta^2(\alpha^4 + \beta^2)) + \mu\kappa^2}. \tag{10}$$

The asymptotics is now linear. Higher approximations are constructed in a similar manner. For example to incorporate two resonances in the fit we can write

$$\lambda^{[4/1]}(\kappa) = \lambda_0 \frac{(\kappa^2 + 2\alpha^2\kappa + \alpha^4 + \beta^2)(\kappa^2 + 2\gamma^2\kappa + \gamma^4 + \delta^2)}{(\alpha^4 + \beta^2)(\gamma^4 + \delta^2)(1 + \mu\kappa)}. \tag{11}$$

The $\lambda^{[4/1]}$ approximation increases as $\kappa^3$ at large $\kappa$. The question now is which one of the proposed approximations represents the function $\lambda(\kappa)$ optimally?

It is obvious that for a stable and accurate analytical continuation the knowledge of the asymptotic behavior is essential. In the following we prove that for a broad class of potentials and nonzero values of the angular momentum $l$ the function $\lambda(\kappa)$ increases as a second power of $\kappa$ at large $\kappa$.

## 2. The main result

In this part we formulate and prove the main result, i.e. the asymptotic behavior of the coupling function $\lambda(\kappa)$. Let us consider equation (4) but we write $\lambda$ instead of $1+\lambda$ (this shift does not change the asymptotic behaviour) and $t$ instead of $r$ (we work in polar coordinates below and using $r$ would be confusing). So, we rewrite (4) as

$$\psi''(t) = A(t)\psi(t), \qquad A(t) = \frac{l(l+1)}{t^2} + \kappa^2 + \lambda V(t). \tag{P}$$

If $l$ and $V$ are fixed, then for any $\kappa \in \mathbb{R}$ we denote

$$\Lambda(\kappa) = \left\{\lambda \in \mathbb{R} : \exists\, \psi \in C^2((0,+\infty)) \text{ satisfying (P) \& } \psi \not\equiv 0 \text{ \& } \lim_{t\to 0+} \psi(t) = 0 = \lim_{t\to+\infty} \psi(t)\right\}$$

and

$$\lambda(\kappa) = \inf \Lambda(\kappa) \qquad \text{(with } \lambda(\kappa) = +\infty \text{ if } \Lambda(\kappa) \text{ is empty).}$$

**Theorem 1.** *Let $l \in (0,+\infty)$ and let $V : [0,+\infty) \to \mathbb{R}$ be a continuous function satisfying $\lim_{t\to+\infty} V(t) = 0$, $\int_1^{+\infty} V(t)dt < +\infty$, and $-m_0 = \min_{t\geq 0} V(t) < 0$. Denote $C_0 = \frac{1}{m_0}$. Then for every $\kappa_0 > 0$ there exists $C_1 > 0$ such that*

$$C_0\kappa^2 \leq \lambda(\kappa) \leq C_1\kappa^2 \tag{12}$$

*holds for every $\kappa > \kappa_0$.*

*Remark* 1. In fact, the asymptotics of $\lambda(\kappa)$, $\kappa \to +\infty$ is close to $C_0\kappa^2$. More precisely, for any small $\varepsilon > 0$ there exists $\kappa_0$ such that (12) holds for all $\kappa > \kappa_0$ with $C_1 = C_0 + \varepsilon$. We can see this from (18) since we can take $m$ very close to $m_0$ and then $\kappa_0$ so large that

$$C_1 = \frac{1}{m}\left(1 + \frac{l(l+1) + a\omega^2}{a\kappa_0^2}\right) < \frac{1}{m_0} + \varepsilon.$$

### 2.1. Proof of the main result.

We start with two lemmas. The first lemma speaks about the equation $y'' = a(t)y$ with $a(t) < 0$. In this case, the solutions oscillates around zero and the first lemma estimates the speed of these oscillations. The second lemma speaks about the case $a(t) > 0$, in particular about asymptotic behavior of solutions as $t \to +\infty$.

**Lemma 2** (a variant of Sturm's Theorem). *Let $I$ be an interval, $\omega > 0$ and $q : I \to (\omega^2, +\infty)$ be a continuous function. Assume that $y, z : I \to \mathbb{R}$ are solutions to*

$$y'' + q(t)y = 0, \qquad z'' + \omega^2 z = 0, \quad \textit{resp.}$$

*Let $(\sigma,\phi)$, $(\rho,\theta)$ satisfy*

$$\begin{aligned} y(t) &= \sigma(t)\cos\phi(t), & y'(t) &= \omega\sigma(t)\sin\phi(t) \\ z(t) &= \rho(t)\cos\theta(t), & z'(t) &= \omega\rho(t)\sin\theta(t) \end{aligned}$$

*for all $t \in I$.*

*Then $\phi(t) < \phi(t_0) - \omega(t - t_0)$ holds for all $t \in I$, $t > t_0$.*

*Proof.* The equations for angles $\phi$, $\theta$ read

$$\begin{aligned}\phi' &= -\frac{q(t)}{\omega}\cos^2\phi - \omega\sin^2\phi = -\omega - \frac{q(t)-\omega^2}{\omega}\cos^2\phi,\\ \theta' &= -\omega\cos^2\theta - \omega\sin^2\theta = -\omega.\end{aligned} \tag{13}$$

Therefore, $(\theta(t)-\phi(t))' \geq 0$ and the equality holds only in the points where $\cos\phi(t) = 0$. Such points are isolated due to $\phi' \leq -\omega$, so $\theta - \phi$ is increasing on $I$. Hence, $\phi(t) < \phi(t_0) + \theta(t) - \theta(t_0) = \phi(t_0) - \omega(t - t_0)$. □

**Lemma 3** ([14], Corollary XI.9.2)**.** *Let $\mu > 0$ and $\int^{\infty} q(t)dt < +\infty$. Then there exist solutions $u_0$, $u_1$ to*

$$u'' = [\mu^2 + q(t)]u \tag{14}$$

*satisfying*

$$u_0 \sim -\frac{u_0'}{\mu} \sim e^{-\mu t}, \qquad u_1 \sim \frac{u_1'}{\mu} \sim e^{\mu t}$$

*as $t \to +\infty$.*

Obviously, $u_0$, $u_1$ are linearly independent, so any solution to (14) is of the form $au_0 + bu_1$ and there is a one-dimensional subspace of solutions vanishing at $+\infty$. In the proof of the main result we will need that if $q$ depends continuously on a parameter $\lambda$, then the subspace of vanishing solutions depends on $\lambda$ continuously. We formulate the statement precisely in Theorem 4 and we postpone its proof to the next subsection.

**Theorem 4** (Continuous dependence of a stable subspace)**.** *Let us consider a problem*

$$u'' = [\mu^2 + \varphi(t,\lambda)]u \tag{15}$$

*with $\mu > 0$ and $\varphi$ being a continuous function on $(a,+\infty)\times(0,+\infty)$ for some $a \in \mathbb{R}$. Assume that there exists $t_0 > a$ such that for any fixed interval $[c, C] \subset (0,+\infty)$ there exists $\varphi_0 \in L^1((t_0,+\infty))$ such that $|\varphi(t,\lambda)| \leq \varphi_0(t)$ for all $t \geq t_0$ and $\lambda \in [c, C]$.*

*Let $\lambda_n \to \lambda_0 > 0$, $T > a$ and let $u_n$, $n = 0,1,2,\ldots$ be non-zero solutions to* (15) *with $\lambda = \lambda_n$ respectively and $\lim_{t\to+\infty} u_n(t) = 0$. Let $\omega > 0$. If $\rho_n$, $\theta_n$ are such that $u_n(T) = \rho_n\cos\theta_n$, $u_n'(T) = \omega\rho_n\sin\theta_n$. Then $\lim_{n\to\infty}\theta_n = \theta_0$ (mod $2\pi$).*

Let us now prove Theorem 1.

*Proof of Theorem 1.* First of all, let $\kappa$, $\lambda \in \mathbb{R}$, $\kappa > 0$ be arbitrary. We observe that the equation (P) is linear of second order with $A$ being a continuous function on $(0,+\infty)$, so for every $t_0 > 0$ and every $\psi_0, \psi_1 \in \mathbb{R}$ there exists a unique solution satisfying $\psi(t_0) = \psi_0$, $\psi'(t_0) = \psi_1$ and the solution is defined on $(0,+\infty)$. Moreover, the set of all solutions to (P) forms a linear space of dimension 2.

It follows from Lemma 3 with $\mu = \kappa^2$ and $q(t) = \frac{1}{t^2}l(l+1) + \lambda V(t)$ that there exists a non-zero solution $\psi_\infty$ to (P) with $\lim_{t\to+\infty}\psi_\infty(t) = 0$ (and obviously all multiples of $\psi_\infty$

have this property). Let us now investigate behavior of solutions at zero. We substitute $\omega(s) = \psi(e^{-s})$, then

$$\begin{aligned}\omega'(s) &= -e^{-s}\psi'(e^{-s}),\\ \omega''(s) &= e^{-2s}\psi''(e^{-s}) + e^{-s}\psi'(e^{-s})\end{aligned}$$

and the equation for $\omega$ reads

$$\begin{aligned}\omega''(s) &= e^{-2s}\left(\frac{l(l+1)}{e^{-2s}} + \kappa^2 + \lambda V(e^{-s})\right)\psi(e^{-s}) + e^{-s}\psi'(e^{-s})\\ &= \left(l(l+1) + \kappa^2 e^{-2s} + \lambda V(e^{-s})e^{-2s}\right)\omega(s) - \omega'(s)\end{aligned}$$

i.e.,

$$\omega''(s) + \omega'(s) - \left(l(l+1) + \kappa^2 e^{-2s} + \lambda V(e^{-s})e^{-2s}\right)\omega(s) = 0.$$

Denoting $u(s) = e^{\frac{1}{2}s}\omega(s)$ we obtain

$$\begin{aligned}u''(s) &= e^{\frac{1}{2}s}\left(\omega''(s) + \omega'(s) + \frac{1}{4}\omega(s)\right)\\ &= e^{\frac{1}{2}s}\left(\left(l(l+1) + \kappa^2 e^{-2s} + \lambda V(e^{-s})e^{-2s}\right)\omega(s) + \frac{1}{4}\omega(s)\right),\end{aligned}$$

i.e.,

$$u''(s) = \left(l(l+1) + \frac{1}{4} + \kappa^2 e^{-2s} + \lambda V(e^{-s})e^{-2s}\right)u(s). \tag{16}$$

Now, we can apply Lemma 3 with $\lambda = \sqrt{\frac{1}{4} + l(l+1)}$ and $q(s) = \kappa^2 e^{-2s} + \lambda V(e^{-s})e^{-2s}$ (which is integrable at $+\infty$ since $V$ is bounded in a neighborhood of zero) and we get solutions

$$\omega_0(s) = e^{-\frac{1}{2}s}u_0(s) \sim e^{\left(-\sqrt{\frac{1}{4}+l(l+1)}-\frac{1}{2}\right)s}, \quad \omega_1(s) = e^{\frac{1}{2}s}u_1(s) \sim e^{\left(-\sqrt{\frac{1}{4}+l(l+1)}-\frac{1}{2}\right)s}$$

as $s \to +\infty$. Let us denote $\psi_0(t) = \omega_0(-\ln t)$. Then $\lim_{t\to 0+}\psi_0(t) = 0$ (and obviously all multiples of $\psi_0$ have this poperty).

We are looking for solutions vanishing simultaneously at zero and infinity, so we would like to have $\psi_\infty = c\psi_0$ for some $c \in \mathbb{R}$. By uniquenes of solutions, it is enough to show that $\psi_\infty(t_1) = c\psi_0(t_1)$ and $\psi'_\infty(t_1) = c\psi'_0(t_1)$ for one (arbitrary) $t_1 \in (0, +\infty)$, which means $\phi_0(t_1) = \phi_\infty(t_1) + 2n\pi$ where $n$ is an integer and $(\rho_0, \phi_0)$, resp. $(\rho_\infty, \phi_\infty)$ are representations of $(\psi_0, \psi'_0)$, resp. $(\psi_\infty, \psi'_\infty)$ in the generalized polar coordinates

$$\begin{aligned}\psi_0 &= \rho_0\cos\phi_0, & \psi'_0 &= \omega\rho_0\sin\phi_0\\ \psi_\infty &= \rho_\infty\cos\phi_\infty, & \psi'_\infty &= \omega\rho_\infty\sin\phi_\infty\end{aligned} \tag{17}$$

(the value of $\omega > 0$ is set below and it depends on the potential $V$ only).

Since $\min_{t\in[0,+\infty)} V(t) < 0$, there exist $m > 0$ and an interval $[a, b]$ (with $0 < a < b < +\infty$) such that $V(t) < -m$ on $[a, b]$. Let us study the problem (P) in the generalized polar coordinates (17) with $\omega = \frac{2\pi}{b-a}$ on the interval $I = [a, b]$. Put $\alpha_0 = \phi_0(a) \in [0, 2\pi)$ and, since $\phi_\infty(b)$ is determined uniquely up to the period $2\pi$, we may choose $\alpha_1 = \phi_\infty(b)$ in such a way that $\alpha_0 > \alpha_1 \geq \alpha_0 - 2\pi$. We show that for large $\lambda$, $\phi_0(b) < \phi_\infty(b)$ and for small $\lambda$ the opposite inequality holds. Further, we show that the dependence of $\phi_0(b)$ and $\phi_\infty(b)$ on $\lambda$ is continuous. Then we conclude that there exists a $\lambda$ between the upper and lower bound for which $\phi_0(b) = \phi_\infty(b)$, and thus we find a solution vanishing at zero and also at infinity.

Let us denote

$$\bar{\lambda}(\kappa) = \frac{1}{m}\left(\frac{l(l+1)}{a^2} + \kappa^2 + \omega^2\right)$$

Then for $\lambda = \bar{\lambda}(\kappa)$ and all $t \in [a, b]$ we have

$$A(t) = \frac{l(l+1)}{t^2} + \kappa^2 + \bar{\lambda}(\kappa)V(t) < \frac{l(l+1)}{a^2} + \kappa^2 - \bar{\lambda}(\kappa)m = -\omega^2.$$

Now, we can apply Lemma 2 with $y(t) = \psi_0(t)$, $q(t) = -A(t) > \omega^2$ and $t_0 = a$. Lemma 2 yields $\phi_0(b) < \phi_0(a) - \omega(b - a) = \alpha_0 - 2\pi \leq \alpha_1 = \phi_\infty(b)$.

On the other hand, let $-m_0$ be the minimum of $V$ on $(0, +\infty)$ and

$$\underline{\lambda}(\kappa) = \frac{\kappa^2}{m_0}.$$

Then for any $\lambda \in \left[0, \underline{\lambda}(\kappa)\right]$ and all $t > 0$ we have

$$A(t) = \frac{l(l+1)}{t^2} + \kappa^2 + \lambda V(t) > \kappa^2 - \lambda m_0 \geq 0.$$

Therefore, positive solutions to (P) are convex and negative solutions are concave. It follows that $\phi_0 \in (0, \frac{\pi}{2})$ for all $t > 0$ or $\phi_0 \in (\pi, \frac{3\pi}{2})$ for all $t > 0$ and $\phi_\infty \in (\frac{\pi}{2}, \pi)$ for all $t > 0$ or $\phi_\infty \in (\frac{3\pi}{2}, 2\pi)$ for all $t > 0$. Since we have chosen $\phi_0(a)$ and $\phi_\infty(b)$ such that $\phi_0(a) > \phi_\infty(b)$, we have $\phi_0(b) > \phi_\infty(b)$ ($\phi_0$ stays in the same segment for all $t$). As a consequence, equality $\phi_0(b) = \phi_\infty(b)$ cannot occur for $\lambda \in \left[0, \underline{\lambda}(\kappa)\right]$, so $\lambda(\kappa) = \inf \Lambda(\kappa) > \underline{\lambda}(\kappa)$.

If $\phi_\infty(b)$ and $\phi_0(b)$ depend continuously on $\lambda$, then we have existence of the desired $\lambda \in \left[\underline{\lambda}(\kappa), \bar{\lambda}(\kappa)\right]$ for which $\phi_0(b) = \phi_\infty(b)$, which implies that $\lambda(\kappa) = \inf \Lambda(\kappa)$ satisfies

$$\frac{\kappa^2}{m_0} = \underline{\lambda}(\kappa) \leq \lambda(\kappa) \leq \bar{\lambda}(\kappa) = \frac{\bar{\lambda}(\kappa)}{\kappa^2}\kappa^2,$$

so the statement of the theorem is proved with $C_0 = \frac{1}{m_0}$ and

$$C_1 = \sup_{\kappa \in [\kappa_0, +\infty)} \frac{\bar{\lambda}(\kappa)}{\kappa^2} = \frac{1}{m} \sup_{\kappa \in [\kappa_0, +\infty)} \left(1 + \frac{l(l+1) + a\omega^2}{a\kappa^2}\right) = \frac{1}{m}\left(1 + \frac{l(l+1) + a\omega^2}{a\kappa_0^2}\right). \tag{18}$$

To prove the continuous dependence we apply Theorem 4. In case of $\phi_\infty$, we rewrite (P) in the form of (15) with $\varphi(t, \lambda) = \lambda V(t)$, which is obviously a continuous function of two variables and $|\varphi(t, \lambda)| \leq \varphi_0(t)$ holds with $\varphi_0 = C|V(t)|$ (which is integrable on $(a, +\infty)$) for all $\lambda \in [c, C] \subset (0, +\infty)$. So, Theorem 4 can be applied and $\phi_\infty(b)$ depends continuously on $\lambda$. In case of $\phi_0$, we apply Theorem 4 to equation (16). In this case, we have $\varphi(t, \lambda) = \kappa^2 e^{-2t} + \lambda V(e^{-t})e^{-2t}$ which is again a continuous function of two variables and $|\varphi(t,\lambda)| \leq \varphi_0(t)$ holds with $\varphi_0(t) = e^{-2t}(\kappa^2 + C|V(0)|)$ for all $\lambda \in [c, C] \subset (0, +\infty)$. Therefore, by Theorem 4, the angle (in generalized polar coordinates) corresponding to the vector $(u_0(T)), u_0'(T))$ for $T = -\ln(b)$ depends continuously on $\lambda$. Since the transformation $(u_0(T), u_0'(T)) \mapsto (\psi_0(e^{-T}), \psi_0'(e^{-T}))$ is linear and continuous, also the angle of $(\psi_0(e^{-T}), \psi_0'(e^{-T}))$ (this angle is exactly $\phi_0(b)$) depends continuously on $\lambda$. □

2.2. **Proof of Theorem 4.** In this section we prove Theorem 4 in a sequence of lemmas. We assume throughout this section that assumptions of Theorem 4 hold.

First observe that every $\lambda > 0$ the function $\varphi(\cdot, \lambda)$ belongs to $L^1((1, +\infty))$, so by [14, Theorem X.17.2] there exist solutions $u_0$, $u_1$ to (15) satisfying

$$u_0(t) = e^{-\mu t}[1 + o(1)], \qquad u_0'(t) = e^{-\mu t}[-\mu + o(1)],$$
$$u_1(t) = e^{\mu t}[1 + o(1)], \qquad u_1'(t) = e^{\mu t}[\mu + o(1)].$$

Consequently, any solution to (15) is of the form $(a + o(1))e^{\mu t} + (b + o(1))e^{-\mu t}$. It follows

**Lemma 5.** *For any $b \in \mathbb{R}$ there exists a unique solution $u$ to* (15) *satisfying* $\lim_{t\to+\infty} e^{\mu t}u(t) = b$ *(it is the solution $bu_0$).*

Further, [14, proof of Lemma X.4.3] implies explicit estimates of the terms $o(1)$ in the above expressions. Let us reformulate (15) to see how [14, Lemma X.4.3] can be applied. First, we write (15) as a first order system

$$U' = \begin{pmatrix} 0 & 1 \\ \mu^2 & 0 \end{pmatrix} U + \begin{pmatrix} 0 & 0 \\ \varphi(t,\lambda) & 0 \end{pmatrix} U$$

Further, we have

$$\begin{pmatrix} 0 & 1 \\ \mu^2 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -\mu & \mu \end{pmatrix} \begin{pmatrix} -\mu & 0 \\ 0 & \mu \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{1}{2\mu} \\ \frac{1}{2} & \frac{1}{2\mu} \end{pmatrix} = CJC^{-1}.$$

Then substitution $V(t) = e^{\mu t}C^{-1}U(t)$ yields

$$V' = \begin{pmatrix} 0 & 0 \\ 0 & 2\mu \end{pmatrix} V + \frac{1}{2\mu}\varphi(t,\lambda) \begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix} V \tag{19}$$

Assuming $V = (y, z)^T$ and adding one more (independent) equation $x' = -x$ we are in the situation of [14, Lemma X.4.3] with $\xi = (x, y, z)^T$, $A_1 = -1$, $A_2 = 0$, $A_3 = 2\mu$, $F_1 \equiv 0$, $F_2(t, \xi, \lambda) = -\frac{1}{2\mu}\varphi(t,\lambda)(y + z) = -F_3(t, \xi, \lambda)$. We use assumptions on $\phi(t, \lambda)$ to get

$$\|F(t, \xi, \lambda)\| \leq \frac{1}{\mu}|\varphi(t,\lambda)||y + z| \leq \frac{1}{\mu}\varphi_0(t)\|\xi\|,$$

so $\psi_0 = \frac{1}{\mu}\varphi_0(t)$ satisfies the assumptions of [14, Lemma X.4.3] for any $\lambda \in [c, C]$. By [14, Lemma X.4.3] for any $y_\infty$ sufficiently small we find a solution $V$ to (19) with $\lim_{t\to+\infty} V(t) = (y_\infty, 0)^T$. Moreover, [14, proof of Lemma X.4.3] shows that

$$|y(t) - y_\infty| \leq 7|y_\infty| \int_t^\infty \psi_0(s)\mathrm{d}s, \quad |z(t)| \leq 7\tau(t)|y(t)|, \quad \text{for } t \geq t_0 \tag{20}$$

where $t_0$, $\tau(t)$ are independent of $\lambda$ (they depend only on $\psi_0$) and $\lim_{t\to+\infty}\tau(t) = 0$. Since our problem si linear, the assertion is also valid for large values of $y_\infty$. Inequalities (20) yields uniform (in $\lambda$) estimates of $\|V(t) - (y_\infty, 0)^T\|$ and consequently also for solutions $u$ of (15). In particular, we have

**Lemma 6.** *Let $y_\infty \in \mathbb{R}$ and $C > c > 0$. For $\lambda \in [c, C]$ let $u_\lambda$ denote the unique solution of* (15) *with $\lim_{t\to+\infty} e^{\mu t}u_\lambda(t) = y_\infty$. There exists $T > a$ and $K : [T, +\infty) \to (0, +\infty)$ with $\lim_{t\to+\infty} K(t) = 0$ such that*

$$|e^{\mu t}u_\lambda(t) - y_\infty| + |e^{\mu t}u'_\lambda(t) + \mu y_\infty| \le K(t) \quad \textit{for } t \ge T$$

*for all $\lambda \in [c, C]$. In particular, $\lim_{t\to+\infty} e^{\mu t}u'_\lambda(t) = -\mu y_\infty$.*

*Proof.* By the previous paragraph, for any $\lambda \in [c, C]$ there exists a solution $V = V_\lambda$ to (19) satisfying (20). If $T \ge t_0$ ($t_0$ from (20)) is so large that $\int_T^{+\infty} \psi_0(s)\mathrm{d}s \le \frac{1}{7}$, then for $t \ge T$ we have $|y(t) - y_\infty| \le |y_\infty|$, e.g. $|y(t)| \le 2|y_\infty|$ and $|z(t)| \le 14\tau(t)|y_\infty|$. Therefore,

$$|y(t) - y_\infty| + |z(t)| \le 7|y_\infty| \left( \int_t^{+\infty} \psi_0(s)\mathrm{d}s + 2\tau(t) \right)$$

Then the corresponding

$$\begin{pmatrix} u_\lambda(t) \\ u'_\lambda(t) \end{pmatrix} = U(t) = e^{-\mu t}CV(t) = e^{-\mu t} \begin{pmatrix} y(t) + z(t) \\ -\mu y(t) + \mu z(t) \end{pmatrix}$$

satisfies

$$|e^{\mu t}u_\lambda(t) - y_\infty| = |y(t) + z(t) - y_\infty| \le 7|y_\infty| \left( \int_t^{+\infty} \psi_0(s)\mathrm{d}s + 2\tau(t) \right)$$

and

$$|e^{\mu t}u'_\lambda(t) + \mu y_\infty| = \mu|y_\infty - y(t) + z(t)| \le 7\mu|y_\infty| \left( \int_t^{+\infty} \psi_0(s)\mathrm{d}s + 2\tau(t) \right)$$

and the Lemma is proved with $K(t) = 7(1+\mu)|y_\infty| \left( \int_t^{+\infty} \psi_0(s)\mathrm{d}s + 2\tau(t) \right) \to 0$. $\square$

**Lemma 7.** *Let $\lambda_n \to \lambda_0 > 0$ and let $u_n$ be a solution to* (15) *with $\lambda = \lambda_n$ satisfying $\lim_{t\to+\infty} e^{\mu t}u_n(t) = 1$. There exists $T > a$ such that for every $t_0 > T$ there exists $u_0$ such that $\lim_{n\to\infty} u_n(t_0) = u_0$ and the solution $u$ of* (15) *with $\lambda = \lambda_0$ and $u(t_0) = u_0$ satisfies $\lim_{t\to+\infty} e^{\mu t}u(t) = 1$. Moreover, $\lim_{n\to\infty} u'_n(t_0) = u'(t_0)$.*

*Proof.* Since $\lambda_n \to \lambda_0 > 0$ we can fix $C > c > 0$ and $n_0$ such that $\lambda_n \in [c, C]$ for all $n \ge n_0$. Let us set $y_\infty = 1$ and apply Lemma 6 to obtain $\|e^{\mu t}u_n(t) - 1\| \le K(t)$ for $t \ge T$. Let us fix $t_0 \ge T$.

1st step. Let us first assume that $\lim_{n\to\infty} u_n(t_0) = u_0$. If the solution $u$ from the lemma does not satisfy $\lim_{t\to+\infty} e^{\mu t}u(t) = 1$, there is $\varepsilon > 0$ and a sequence $t_n \nearrow +\infty$ such that $\|e^{\mu t_n}u(t_n) - 1\| > 2\varepsilon$. However, for $t_m$ large enough we have $\varepsilon > K(t_m)$, i.e. $\|e^{\mu t_m}u(t_m) - 1\| > K(t_m) + \varepsilon$. On the other hand, $\|e^{\mu t_m}u_n(t_m) - 1\| \le K(t_m)$ for all $n \ge n_0$, which is a contradiction since $u_n \to u$ uniformly on compact intervals due to continuous dependence on initial values and parameters.

2nd step. Let us now assume, that $\lim_{n\to\infty} u_n(t_0)$ does not exist. Since the sequence $u_n(t_0)$ is bounded (due to $\|e^{\mu t}u_n(t)-1\| \le K(t)$), there exist two subsequences with different limits $u_0 \neq \tilde{u}_0$. Applying the 1st step to these subsequences we conclude that solutions $u$, $\tilde{u}$ to (15) with $\lambda = \lambda_0$ and initial values $u(t_0) = u_0$, resp. $\tilde{u}(t_0) = \tilde{u}_0$ satisfy $\lim_{t\to+\infty} e^{\mu t}u(t) = 1 = \lim_{t\to+\infty} e^{\mu t}\tilde{u}(t)$. However, by Lemma 5 we have $u = \tilde{u}$, so $u_0 = \tilde{u}_0$. This is a contradiction.

By Lemma 6, we have $\lim_{t\to+\infty} e^{\mu t}u_n'(t) = -\mu$ and we can use the same arguments as above for derivatives $u_n'$, $u'$ instead of $u_n$, $u$ to get $\lim_{n\to\infty} u_n'(t_0) = u'(t_0)$. □

*Proof of Theorem 4.* For any fixed $\lambda > 0$ and $T > a$ there is a one-dimensional space of solutions with the property $\lim_{t\to+\infty} u_n(t) = 0$. So, $u_n$ is not uniquely determined but $\theta_n$ is unique (up to a multiple of $\pi$). So, we can without loss of generality assume that $\lim_{t\to+\infty} e^{\mu t}u_n(t) = 1$, $n = 0, 1, 2, \ldots$. By Lemma 7 we have $u_n(t_0) \to u_0(t_0)$, $u_n'(t_0) \to u_0'(t_0)$ for any $t_0$ large enough. Continuous dependence on initial conditions and parameters ($u_n(t_0) \to u_0(t_0)$, $u_n'(t_0) \to u_0'(t_0)$ and $\lambda_n \to \lambda_0$) then implies $u_n(T) \to u_0(T)$, $u_n'(T) \to u_0'(T)$ for any $T > a$. Since $(u_0(T), u_0'(T)) \neq (0, 0)$ (by uniqueness of solutions), convergence of the angles $\theta_n \to \theta_0$ in generalized polar coordinates follows. □

## 3. Summary and results

In the applications of the RAC method and its variant the ACCC method, see for example: [11], [12], [13], we observed that best results are obtained with approximations satisfying the $\kappa^2$ behavior at $\kappa \to \infty$. The result obtained in this work puts our experimental experience on a firmer footing. The approximations $\lambda^{[3/1]}(\kappa)$ (Eq. (9)), $\lambda^{[4/2]}(\kappa)$, $\lambda^{[5/3]}(\kappa)$, etc. are recommended and the approximations $\lambda^{[3/2]}(\kappa)$ (Eq. (10)), $\lambda^{[4/1]}(\kappa)$ (Eq. (11)), etc. should be treated with caution because of their false asymptotic behavior.

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