Critical domain of coupling constants of short-range potentials

2001 J. Phys. A: Math. Gen. 34 903

(http://iopscience.iop.org/0305-4470/34/4/315)

J. Phys. A: Math. Gen. **34** (2001) 903–917 www.iop.org/Journals/ja PII: S0305-4470(01)15622-2

Critical domain of coupling constants of short-range potentials

J Stanojević[1], M Božić[1] and R J Lombard[2]

[1] Institute of Physics, PO Box 57, 11001 Belgrade, Yugoslavia
[2] Groupe de Physique théorique, Institute de Physique Nucléaire, 91406 Orsay Cedex, France

Received 17 July 2000, in final form 6 October 2000

Abstract
In this paper, we consider three-dimensional short-range potentials of several components, i.e. depending on several coupling constants. For N components, the critical domain is defined as the $(N-1)$-dimensional surface separating the regions with and without a bound state in the space of the coupling constants. It is shown that the problem of finding the critical domain can be solved by generalizing the methods established for the determination of the critical coupling constant in the case of a single-component potential. Applications are made for the truncated harmonic oscillator and the square-well potentials with a spin–orbit interaction of the Thomas form.

PACS number: 0365G

1. Introduction

In the three-dimensional space, considering short-range potentials $-\lambda V(r)$ (with $V(r) > 0$), it is well known that the existence of a bound state is governed by the critical value of the coupling constant λ_c [1]. To be specific, short-range potentials are defined so that they possess at most a finite number of bound states. Thus, we consider potentials which decrease fast enough to become negligible beyond a finite radius ($\lim_{r\to\infty} r^2 V(r) = 0$), and we discard cases with a singularity at the origin. The critical value λ_c is an important characteristic of the potential. Two different methods have been investigated for its determination [2, 3]. The first one is based on the Green function technique (GFT) [2], while the second relies on the Jost function at zero energy (JFM) [3]. Furthermore, the variation of the energy eigenvalue near the critical λ_c has been studied [4, 5]. This variation obeys a power law, the power being dependent on the orbital angular momentum ℓ.

Real physical potentials could have several components and thus depend on several parameters. This paper considers potentials of the form $U(r; \boldsymbol{\lambda}) = -\sum_{i=1}^{N} \lambda_i V_i(r)$, where all $V_i(r)$ components are short-range potentials. Then, the problem of the bound state existence reduces to the determination of a critical domain $\boldsymbol{\lambda}_c \stackrel{\text{def}}{=} (\lambda_{1c}, \lambda_{2c}, \ldots, \lambda_{Nc})$, which delineates two regions in the parameter space. In one region at least one bound state exists, while the other contains no bound state. Note that for a potential with N components, the critical domain

$\boldsymbol{\lambda}_c$ consists in an $(N-1)$-dimensional surface in the parameter space. It reduces to a curve splitting the plane in the two-component case.

The paper is organized as follows. We describe, in section 2, general properties of the critical domain of the parameter space, and two procedures are developed to generalize methods used in the single-component case. In section 3, one of these procedures is further investigated in connection with JFM. Two typical examples are treated in section 4: critical domains (curves) are determined for the square well and the truncated harmonic potentials with a spin–orbit component of the Thomas form.

2. General properties of a critical domain of coupling constants

We consider short-range potentials $U(r;\boldsymbol{\lambda}) = -\sum_i^N \lambda_i V_i(r)$ depending on a set $\boldsymbol{\lambda} \equiv \{\lambda_i\}$ of coupling constants, with $V_i(r) > 0$. The corresponding Hamiltonian reads

$$H(\boldsymbol{r};\boldsymbol{\lambda}) = T + U(r;\boldsymbol{\lambda}). \tag{1}$$

Bound state wavefunctions $\psi_n(\boldsymbol{r},\boldsymbol{\lambda})$ are solutions of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U(r;\boldsymbol{\lambda})\right)\psi_n(\boldsymbol{r},\boldsymbol{\lambda}) = E_n(\boldsymbol{\lambda})\psi_n(\boldsymbol{r},\boldsymbol{\lambda}) \tag{2}$$

with eigenvalues $E_n(\boldsymbol{\lambda}) \leqslant 0$. For short-range potentials, positive energy solutions are not square integrable, and the radial part is a linear superposition of $\psi_\pm(\boldsymbol{r}) \sim \exp(\pm \mathrm{i} r\sqrt{2mE_n(\boldsymbol{\lambda})/\hbar^2})/r$. Therefore, these solutions do not represent bound states [6].

In general, the Hamiltonian (1) possesses bound states only in a certain region of the parameter space. Therefore, for each value of the quantum numbers, that we loosely denote by n, the whole parameter space $\Lambda \ni (\lambda_1, \lambda_2, \ldots, \lambda_N)$ is divided into two subspaces, Λ_b^n and Λ_u^n. In Λ_b^n the nth bound state exists, whereas it is absent in Λ_u^n. It is clear that the point $(\lambda_i = 0, \forall i) \in \Lambda_u^n$. The critical domain of parameters $\mathcal{L}_n^c$ is the border between the subspaces Λ_b^n and Λ_u^n. If n is the ground state, its critical domain represents at the same time the threshold conditions for the appearance of a bound state.

In the case of a single component, the JFM determination of λ_c is achieved by setting $E = 0$ in the corresponding Schrödinger equation [4]. For several components, the critical domain $\mathcal{L}_n^c$ is determined similarly by the relation

$$E_n(\boldsymbol{\lambda}) = 0. \tag{3}$$

This may be shown by using the Hellman–Feynman theorem [7, 8], according to which, the variation of the eigenvalues with respect to parameters

$$\delta E_n(\boldsymbol{\lambda}) = \frac{\partial E_n(\boldsymbol{\lambda})}{\partial \lambda_i}\delta\lambda_i \tag{4}$$

is linked to the variation of the Hamiltonian

$$\delta H(\boldsymbol{r};\boldsymbol{\lambda}) = \delta U(r;\boldsymbol{\lambda}) = \sum_i \frac{\partial U(r;\boldsymbol{\lambda})}{\partial \lambda_i}\delta\lambda_i = -\sum_i V_i(r)\delta\lambda_i \tag{5}$$

through

$$\delta E_n(\boldsymbol{\lambda}) = \frac{\int |\psi_n(\boldsymbol{r},\boldsymbol{\lambda})|^2 \delta U(r;\boldsymbol{\lambda})\,\mathrm{d}\vec{r}}{\int |\psi_n(\boldsymbol{r},\boldsymbol{\lambda})|^2\,\mathrm{d}\vec{r}} = -\sum_i \langle V_i\rangle_n\,\delta\lambda_i. \tag{6}$$

Here

$$\langle V_i \rangle_n = \frac{\int |\psi_n(\boldsymbol{r}, \boldsymbol{\lambda})|^2 V_i(r)\, \mathrm{d}\vec{r}}{\int |\psi_n(\boldsymbol{r}, \boldsymbol{\lambda})|^2\, \mathrm{d}\vec{r}}.$$

Therefore,

$$\frac{\partial E_n(\boldsymbol{\lambda})}{\partial \lambda_i} = - \langle V_i \rangle_n . \tag{7}$$

If $V_i(r) > 0,\ \forall r$, then $\langle V_i \rangle_n > 0$ and

$$\frac{\partial E_n(\boldsymbol{\lambda})}{\partial \lambda_i} < 0$$

are surely satisfied. We conclude that the function $E_n(\boldsymbol{\lambda})$, $\boldsymbol{\lambda} \in \Lambda_b^n$ has no local maxima or minima. Therefore, by increasing any λ_i, keeping constant all λ_j $j \neq i$, $E_n(\boldsymbol{\lambda})$ decreases and we enter further into the region Λ_b^n. By decreasing any λ_i, keeping constant all λ_j $j \neq i$, $E_n(\boldsymbol{\lambda})$ increases, approaching $E_n(\boldsymbol{\lambda}) = 0$. So, the critical domain $\mathcal{L}_n^c$ is determined by equation (3).

Considering the domain $\mathcal{L}_n$ determined by $E_n(\boldsymbol{\lambda}) =$ constant, the following property has to be underlined. By varying two parameters λ_i and λ_j inside $\mathcal{L}_n$, we find

$$\frac{\partial E_n}{\partial \lambda_i}\delta\lambda_i + \frac{\partial E_n}{\partial \lambda_j}\delta\lambda_j = 0 \tag{8}$$

i.e.

$$\langle V_i \rangle_n \delta\lambda_i + \left\langle V_j \right\rangle_n \delta\lambda_j = 0. \tag{9}$$

In $\mathcal{L}_n$, any λ_i is therefore a function of the other parameters, i.e. $\lambda_i = \lambda_i(\lambda_1, \ldots, \lambda_{i-1}, \lambda_{i+1}, \ldots, \lambda_N)$. By combining equation (9) with the positivity of $\langle V_i \rangle_n$ and $\left\langle V_j \right\rangle_n$ leads to

$$\frac{\partial \lambda_i}{\partial \lambda_j} = -\frac{\left\langle V_j \right\rangle_n}{\langle V_i \rangle_n} < 0. \tag{10}$$

The latter equation shows that the function $\lambda_i = \lambda_i(\lambda_1, \ldots, \lambda_{i-1}, \lambda_{i+1}, \ldots, \lambda_N)$ is a monotonically decreasing function of all $\lambda_j,\ j \neq i$. Obviously, the critical domain $\mathcal{L}_n^c$, determined by $E_n(\boldsymbol{\lambda}) = 0$, possesses the same property.

To any method designed to obtain the critical coupling constant in the case of a single component, we propose two procedures for its extension to the determination of the critical domain of a multiple-component potential.

(a) In the first procedure, we introduce an auxiliary potential, $U'(r; g, \boldsymbol{\lambda}) = gU(r; \boldsymbol{\lambda}) = -g\left(\sum_{i=1}^N \lambda_i V_i(r)\right)$, with $N + 1$ parameters. Here, the global parameter g takes the role of λ of a single-component potential, whereas $-U(r; \boldsymbol{\lambda}) = \sum_{i=1}^N \lambda_i V_i(r)$ plays the role of $V(r)$. For any arbitrary set $\boldsymbol{\lambda}$, we can obtain the critical value $g_c(\boldsymbol{\lambda})$ by applying any method devoted to the single-component case. By generating an arbitrarily large ensemble of sets $\boldsymbol{\lambda}$, we build the function $g_c(\boldsymbol{\lambda})$. It is obviously assumed that $U(r; \boldsymbol{\lambda})$ satisfies the condition imposed on $V(r)$ in the chosen method. The equation

$$g = g_c(\boldsymbol{\lambda}) \tag{11}$$

determines the critical domain of the auxiliary potential $U'(r; g, \boldsymbol{\lambda})$. For the original potential $U(r; \boldsymbol{\lambda})$ the equation reads

$$1 = g_c(\boldsymbol{\lambda}). \tag{12}$$

In general, instead of equation (11), where g_c is given explicitly, we will obtain a certain implicit relation

$$F(g, \boldsymbol{\lambda}) = 0 \tag{13}$$

so that the equation of the critical domain of the original potential reads

$$F(g = 1, \boldsymbol{\lambda}) = 0. \tag{14}$$

(b) In the second procedure, we replace the set $\boldsymbol{\lambda}$ by $\left(\lambda, \boldsymbol{\beta} \stackrel{\text{def}}{=} (\beta_1, \beta_2, \ldots, \beta_{N-1})\right)$, and we define $W(r; \boldsymbol{\beta})$ so that

$$\lambda W(r; \boldsymbol{\beta}) \equiv \sum_{i=1}^{N} \lambda_i V_i(r). \tag{15}$$

Similarly to the previous procedure, an ensemble of arbitrary sets $\boldsymbol{\beta}$ determine an ensemble of $\lambda_c(\boldsymbol{\beta})$. Again any method designed for λ_c can be used, assuming that $W(r; \boldsymbol{\beta})$ satisfies the conditions imposed upon $V(r)$. However, it may happen that for some specific sets $\boldsymbol{\beta}$, no critical value $\lambda_c(\boldsymbol{\beta})$ exists, and these sets must be excluded. In this way, we determine the function $\lambda_c(\boldsymbol{\beta})$, for all values of $\boldsymbol{\beta}$ for which a critical value $\lambda_c(\boldsymbol{\beta})$ exists. The critical domain consists of all such points $(\lambda_c(\boldsymbol{\beta}), \boldsymbol{\beta})$.

3. The Jost function method

The Jost function method has been applied to the determination of the critical coupling constant of a potential $U(\lambda; r) = -\lambda V(r)$ in [3]. Details concerning the method can be found in this paper. Here we shall recall few points for the sake of completeness. Assuming spherical symmetry, the usual decomposition of the wavefunction on the spherical harmonics

$$\psi(\boldsymbol{r}; \lambda) = \sum_{\ell,m} \frac{\varphi_\ell(r; \lambda)}{r} Y_\ell^m(\Omega) \tag{16}$$

leads to

$$\frac{\mathrm{d}^2\varphi_\ell}{\mathrm{d}r^2} = \left[\frac{2m}{\hbar^2}(-E - \lambda V(r)) + \frac{\ell(\ell+1)}{r^2}\right]\varphi_\ell. \tag{17}$$

It is convenient to consider at first the $\ell = 0$ case.

From here on, we denote $(2m/\hbar^2)\lambda$ by λ. Looking for λ_c, we search for the value of λ, such that

$$-\frac{\mathrm{d}^2\varphi_0}{\mathrm{d}r^2} - \lambda_c V(r)\varphi_0 = 0 \tag{18}$$

with the following constraints: $\varphi_0(r; \lambda_c)$ vanishes at $r = 0$, it is constant asymptotically, and has no node $\varphi_0(r; \lambda_c) \geqslant 0$.

The latter equation is transformed into the Volterra integral equation with the boundary condition $\lim_{r\to\infty} \varphi_0(r; \lambda_c) = 1$

$$\varphi_0(r; \lambda_c) = 1 - \lambda_c \int_r^\infty (r' - r)V(r')\varphi_0(r'; \lambda_c)\,\mathrm{d}r'. \tag{19}$$

Writing $\varphi_0(r; \lambda_c)$ as a series expansion

$$\varphi_0(r; \lambda_c) = \sum_{j=0}^{\infty} \varphi_0^{(j)}(r; \lambda_c). \tag{20}$$

Equation (19) is solved by iteration

$$\begin{aligned}
&\varphi_0^{(0)}(r;\lambda_c) = 1\\
&\varphi_0^{(j)}(r;\lambda_c) = -\lambda_c \int_r^{\infty} (r'-r)V(r')\varphi_0^{(j-1)}(r';\lambda_c)\,\mathrm{d}r'.
\end{aligned} \tag{21}$$

The condition that $\varphi_0(r;\lambda_c)$ vanishes at $r=0$ leads to the equation

$$\varphi_0(0;\lambda_c) = \sum_{j=0}^{\infty}(-1)^j a_j \lambda_c^j = 0 \tag{22}$$

where

$$\begin{aligned}
a_0 &= 1\\
a_1 &= \int_0^{\infty} r_1 V(r_1)\,\mathrm{d}r_1\\
&\vdots\\
a_j &= \int_0^{\infty} r_1 V(r_1)\,\mathrm{d}r_1 \int_{r_1}^{\infty}(r_2-r_1)V(r_2)\,\mathrm{d}r_2 \times \cdots\\
&\qquad \times \int_{r_{j-2}}^{\infty}(r_{j-1}-r_{j-2})V(r_{j-1})\,\mathrm{d}r_{j-1}\int_{r_{j-1}}^{\infty}(r_j-r_{j-1})V(r_j)\,\mathrm{d}r_j.
\end{aligned} \tag{23}$$

Therefore, the determination of the critical value λ_c reduces to the search of a solution of equation (22).

Since $V(r)>0$, the coefficients a_j are subject to the relationship [3]

$$a_j \leqslant \frac{a_{j-1}}{2}M \qquad j \geqslant 2 \tag{24}$$

where $M = \int_0^{\infty}\mathrm{d}r\, rV(r)$. For $\lambda \leqslant 2/M$ the mth-order remainder

$$R_{m+1}(\lambda) \stackrel{\text{def}}{=} \sum_{j=m+1}^{\infty}(-1)^j a_j \lambda^j \tag{25}$$

associated with the mth-order polynomial

$$P_m(\lambda) \stackrel{\text{def}}{=} \sum_{j=0}^{m}(-1)^j a_j \lambda^j \tag{26}$$

fulfils the following relations:

$$\begin{aligned}
&\forall p \geqslant 1 \qquad R_{2p}(\lambda) \geqslant 0\\
&\forall p \qquad\quad\; R_{2p+1}(\lambda) \leqslant 0.
\end{aligned} \tag{27}$$

Provided that $M^2 - 4a_2 \geqslant 0$, it has been shown [3] that the critical value λ_c (solution of equation (22)) satisfies the following sequence of inequalities:

$$\frac{1}{M} = \lambda_1 \leqslant \lambda_3 \leqslant \lambda_c \leqslant \lambda_4 \leqslant \lambda_2 \leqslant \frac{2}{M} \tag{28}$$

where λ_j is a real root of the polynomial $P_j(\lambda)$.

For these polynomials, we prove the following theorem by using mathematical induction.

Theorem. *Provided that $M^2 - 4a_2 \geqslant 0$, $\forall k \geqslant 2$, there exist zeros of the polynomials $P_{2k-3}(\lambda)$, $P_{2k-2}(\lambda)$, $P_{2k-1}(\lambda)$, $P_{2k}(\lambda)$, denoted by λ_{2k-3}, λ_{2k-2}, λ_{2k-1}, λ_{2k}, respectively, so that the following sequence of inequalities is satisfied:*

$$\frac{1}{M} \leqslant \lambda_{2k-3} \leqslant \lambda_{2k-1} \leqslant \lambda_c \leqslant \lambda_{2k} \leqslant \lambda_{2k-2} \leqslant \frac{2}{M}. \tag{29}$$

Here λ_c is the solution of equation (22).

The proof is explicitly given in appendix A.

Therefore, certain zeros of polynomials of odd (even) order determine the lower (upper) bound for λ_c. The interval determined by these bounds decreases with increasing order of the polynomial.

In the case $\ell \neq 0$, the corresponding radial part of the wavefunction for $E = 0$ has to satisfy the equation

$$-\frac{\mathrm{d}^2\varphi_\ell}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2}\varphi_\ell - \lambda_c V(r)\varphi_\ell = 0. \tag{30}$$

After the transformations $r = x^{1/(2\ell+1)}$ and $\varphi_\ell = r^{-\ell}u_\ell$ we obtain

$$-\frac{\mathrm{d}^2u_\ell}{\mathrm{d}x^2} - \frac{\lambda_c}{(2\ell+1)^2}x^{-4\ell/(2\ell+1)}V(x^{1/(2\ell+1)})u_\ell = 0 \tag{31}$$

which is equivalent to the s-wave case.

Consequently, we may apply the same procedure as in the case $\ell = 0$, with the effective potential

$$U_{\text{eff}}(x) \overset{\text{def}}{=} -\frac{\lambda_c}{(2\ell+1)^2}x^{-4\ell/(2\ell+1)}V(x^{1/(2\ell+1)}).$$

It is easily verified that the latter potential is not singular as long as $V(x)$ is not singular, so that the procedure developed for $\ell = 0$ is applicable. The series expansion for the function $u_\ell(r = 0; \lambda_c)$, which corresponds to expansion (22), reads

$$u_\ell(r = 0; \lambda_c) = \sum_{j=0}^{\infty}(-1)^j a_j^{(\ell)}\left(\frac{\lambda_c}{2\ell+1}\right)^j \tag{32}$$

where

$$a_0^{(\ell)} = 1$$

$$a_1^{(\ell)} = \int_0^\infty \mathrm{d}r_1\, r_1 V(r_1)$$

$$\vdots$$

$$\begin{aligned} a_j^{(\ell)} = \int_0^\infty r_1 V(r_1)\,\mathrm{d}r_1 \int_{r_1}^\infty \left(r_2 - r_1\left(\frac{r_1}{r_2}\right)^{2\ell}\right) V(r_2)\,\mathrm{d}r_2 \times \cdots \\ \times \int_{r_{j-2}}^\infty \left(r_{j-1} - r_{j-2}\left(\frac{r_{j-2}}{r_{j-1}}\right)^{2\ell}\right) V(r_{j-1})\,\mathrm{d}r_{j-1} \\ \times \int_{r_{j-1}}^\infty \left(r_j - r_{j-1}\left(\frac{r_{j-1}}{r_j}\right)^{2\ell}\right) V(r_j)\,\mathrm{d}r_j. \end{aligned} \tag{33}$$

In the latter expressions (in which $\ell = 0, 1, 2, \ldots$) $V(r)$ is the original potential.

Turning to the case of a multiple-component potential, the second procedure described in the preceding section is best suitable when applied in connection with the JFM together with the above theorem. Since the JFT method is not applicable to singular potentials, any component of $V_i(r)$ has to be regular.

Accordingly, the parameter set $(\lambda, \boldsymbol{\beta})$ is defined by equation (15), and the polynomials (26) are replaced by

$$P_m(\lambda, \boldsymbol{\beta}) = \sum_{j=0}^{m} (-1)^j a_j(\boldsymbol{\beta}) \lambda^j. \tag{34}$$

The coefficients $a_j(\boldsymbol{\beta})$ are given by

$$\begin{aligned}
a_0(\boldsymbol{\beta}) &= 1 \\
a_1(\boldsymbol{\beta}) &= \int_0^\infty r_1 W(r_1; \boldsymbol{\beta}) \,\mathrm{d}r_1 \\
&\vdots \\
a_j(\boldsymbol{\beta}) &= \int_0^\infty r_1 W(r_1; \boldsymbol{\beta}) \,\mathrm{d}r_1 \int_{r_1}^\infty (r_2 - r_1) W(r_2; \boldsymbol{\beta}) \,\mathrm{d}r_2 \times \cdots \\
&\quad \times \int_{r_{j-2}}^\infty (r_{j-1} - r_{j-2}) W(r_{j-1}; \boldsymbol{\beta}) \,\mathrm{d}r_{j-1} \int_{r_{j-1}}^\infty (r_j - r_{j-1}) W(r_j; \boldsymbol{\beta}) \,\mathrm{d}r_j.
\end{aligned} \tag{35}$$

In the case $\ell \neq 0$, the polynomial (26) and the expressions (33) are generalized to

$$P_m^{(\ell)}(\lambda, \boldsymbol{\beta}) = \sum_{j=0}^{m} (-1)^j a_j^{(\ell)}(\boldsymbol{\beta}) \left(\frac{\lambda}{2\ell + 1}\right)^j \tag{36}$$

where

$$\begin{aligned}
a_0^{(\ell)}(\boldsymbol{\beta}) &= 1 \\
a_1^{(\ell)}(\boldsymbol{\beta}) &= \int_0^\infty r_1 W(r_1; \boldsymbol{\beta}) \,\mathrm{d}r_1 \\
&\vdots \\
a_j^{(\ell)}(\boldsymbol{\beta}) &= \int_0^\infty r_1 W(r_1; \boldsymbol{\beta}) \,\mathrm{d}r_1 \int_{r_1}^\infty \left(r_2 - r_1 \left(\frac{r_1}{r_2}\right)^{2\ell}\right) W(r_2; \boldsymbol{\beta}) \,\mathrm{d}r_2 \times \cdots \\
&\quad \times \int_{r_{j-2}}^\infty \left(r_{j-1} - r_{j-2} \left(\frac{r_{j-2}}{r_{j-1}}\right)^{2\ell}\right) W(r_{j-1}; \boldsymbol{\beta}) \,\mathrm{d}r_{j-1} \\
&\quad \times \int_{r_{j-1}}^\infty \left(r_j - r_{j-1} \left(\frac{r_{j-1}}{r_j}\right)^{2\ell}\right) W(r_j; \boldsymbol{\beta}) \,\mathrm{d}r_j.
\end{aligned} \tag{37}$$

The roots of the polynomials (34) and (36) depend on $\boldsymbol{\beta}$. If $W(r; \boldsymbol{\beta}) \geqslant 0$, the above theorem is valid. The inequalities (29) become inequalities for roots which are functions of $\boldsymbol{\beta}$:

$$\lambda_{2k-3}(\boldsymbol{\beta}) \leqslant \lambda_{2k-1}(\boldsymbol{\beta}) \leqslant \lambda_c(\boldsymbol{\beta}) \leqslant \lambda_{2k}(\boldsymbol{\beta}) \leqslant \lambda_{2k-2}(\boldsymbol{\beta}). \tag{38}$$

Since all $V_i(r) > 0$, the condition $W(r;\beta) \geqslant 0$ implies, in fact, conditions on the values of β_i. In the region of β_i in which the theorem is applicable, we determine the upper and the lower limits of $\lambda_c(\boldsymbol{\beta})$, by using the inequalities (38) and by increasing the value of k step by step.

In the region of β_i in which the roots $\lambda_{2k-1}(\boldsymbol{\beta})$ and $\lambda_{2k}(\boldsymbol{\beta})$ do not satisfy the inequality (38), the concept of lower and upper boundaries loses its meaning. Nevertheless, we are left with approximate evaluations of the critical domain. Indeed, it turns out that for the two examples displayed in the next section, the roots converge to a limit. Thus, the values $\lambda_{2k-1}(\boldsymbol{\beta})$ and $\lambda_{2k}(\boldsymbol{\beta})$ get rapidly close to each other. In such a case, they may be used as an approximation for $\lambda_c(\boldsymbol{\beta})$. Note that the size of the interval between the roots should decrease with increasing k, a point to be verified at each step.

The original parameters λ_i are obtained by substituting $W(r;\beta)$ in the definition of the $a_j^{(\ell)}(\boldsymbol{\beta})$ in equation (37) by the right-hand side of equation (15). It yields

$$P_m^{(\ell)}(\lambda,\boldsymbol{\beta}) = \sum_{j=0}^{m}(-1)^j p_j^{(\ell)}(\boldsymbol{\lambda})\left(\frac{1}{2\ell+1}\right)^j \equiv \mathcal{P}_m^{(\ell)}(\boldsymbol{\lambda}) \tag{39}$$

where

$$p_0^{(\ell)}(\boldsymbol{\lambda}) = 1$$

$$p_1^{(\ell)}(\boldsymbol{\lambda}) = \int_0^\infty r_1\bigg(\sum_{i=1}^{N}\lambda_i V_i(r_1)\bigg)\,\mathrm{d}r_1$$

$$\vdots$$

$$\begin{aligned} p_j^{(\ell)}(\boldsymbol{\lambda}) = {} & \int_0^\infty r_1\bigg(\sum_{i=1}^{N}\lambda_i V_i(r_1)\bigg)\,\mathrm{d}r_1 \int_{r_1}^\infty \left(r_2 - r_1\left(\frac{r_1}{r_2}\right)^{2\ell}\right)\bigg(\sum_{i=1}^{N}\lambda_i V_i(r_2)\bigg)\,\mathrm{d}r_2 \times \cdots \\ & \times \int_{r_{j-2}}^\infty \left(r_{j-1} - r_{j-2}\left(\frac{r_{j-2}}{r_{j-1}}\right)^{2\ell}\right)\bigg(\sum_{i=1}^{N}\lambda_i V_i(r_{j-1})\bigg)\,\mathrm{d}r_{j-1} \\ & \times \int_{r_{j-1}}^\infty \left(r_j - r_{j-1}\left(\frac{r_{j-1}}{r_j}\right)^{2\ell}\right)\bigg(\sum_{i=1}^{N}\lambda_i V_i(r_j)\bigg)\,\mathrm{d}r_j. \end{aligned} \tag{40}$$

The approximate critical set $\boldsymbol{\lambda}_c$ is found by searching the roots of the polynomials

$$\begin{aligned} \mathcal{P}_{2k-1}^{(\ell)}(\boldsymbol{\lambda}) &= 0 \\ \mathcal{P}_{2k}^{(\ell)}(\boldsymbol{\lambda}) &= 0. \end{aligned} \tag{41}$$

Note that equations (40) and (41) can be obtained directly, using the first procedure described in section 2. We start from the equations

$$P_m^{(\ell)}(\lambda) = \sum_{j=0}^{m}(-1)^j a_j^{(\ell)}\left(\frac{\lambda}{2\ell+1}\right)^j = 0 \qquad m = 2k-1 \quad \text{and} \quad m = 2k$$

associated with equation (32). Here the coefficients $a_j^{(\ell)}$ are given by equation (23) (for the $\ell = 0$ case) and by equation (33) (for the $\ell \neq 0$ case). Then we rewrite the latter equation for the potential $U'(r; g, \boldsymbol{\lambda}) = gU(r; \boldsymbol{\lambda}) = -g\left(\sum_{i=1}^{N} \lambda_i V_i(r)\right)$ which contains the auxiliary parameter g. We are left with

$$P_m^{(\ell)'}(g, \boldsymbol{\lambda}) = \sum_{j=0}^{m} (-1)^j p_j^{(\ell)}(\boldsymbol{\lambda}) \left(\frac{g}{2\ell+1}\right)^j = 0 \qquad m = 2k-1 \quad \text{and} \quad m = 2k$$

where $p_j^{(\ell)}(\boldsymbol{\lambda})$ are obtained by substituting $V(r)$ in a_j from equation (23) and $a_j^{(\ell)}$ from equation (33), by $\sum_{i=1}^{N} \lambda_i V_i(r)$. However, these are just the coefficients given by equation (40). At the last step we eliminate g by substituting $g = 1$ into $P_m^{(\ell)'}(g, \boldsymbol{\lambda})$. The result is

$$P_m^{(\ell)'}(g = 1, \boldsymbol{\lambda}) = \mathcal{P}_m^{(\ell)}(\boldsymbol{\lambda}) = 0 \qquad m = 2k-1 \quad \text{and} \quad m = 2k.$$

4. Examples of two-component short-range potentials

For the sake of illustration, the generalized JFM has been applied to the case of two-component potentials. In this respect, the choice of combining a scalar and a spin–orbit term seems particularly interesting. Consequently, our method has been applied to

$$U(r; \boldsymbol{\lambda}) = -\lambda_1 V_1(r) + \lambda_2 \frac{1}{r} \frac{\partial V_1(r)}{\partial r} \vec{\ell} \cdot \vec{s} \tag{42}$$

where the spin–orbit component has a Thomas form. As far as $V_1(r)$ is concerned, two examples have been retained. The two chosen $V_1(r)$ potentials admit analytical solutions, so that the exact critical values can be calculated, allowing a formal test of the lower and upper boundaries, as well as the approximate evaluations in regions of the parameter space where the inequalities (38) do not hold. The analytical solutions are given in appendix B.

4.1. *Truncated harmonic potential with spin–orbit interaction*

In the first example, the potential $V_1(r)$ takes the form

$$V_1(r) = (R^2 - r^2)\Theta(R - r) \tag{43}$$

where $\Theta(R - r)$ is the step function.

The roots of polynomials $\mathcal{P}_5^{(1)}(\boldsymbol{\lambda})$ and $\mathcal{P}_6^{(1)}(\boldsymbol{\lambda})$ have been determined. The resulting curves are plotted in figure 1 for $\ell = 1$, $j = \frac{1}{2}$ and $\ell = 1$, $j = \frac{3}{2}$. These two limits are so close to each other that they are indistinguishable. Moreover, they are practically identical to the exact critical curve determined using exact solutions of the Schrödinger equation.

This example clearly shows that when the roots are becoming close to each other, they accurately approximate the critical curve, whether or not they represent lower and upper boundaries.

Note that the analytic solutions give access to the critical λ_c regardless of the principal quantum number n, whereas the approximate JFM is valid only for the state with no node ($n = 0$, i.e. the states belonging to the lowest Regge trajectory). To yield an insight into how the critical curves behave as a function of n, the cases $n = 0$, 1 and 2 for $\ell = 1$, $j = \frac{1}{2}$ and $\ell = 1$, $j = \frac{3}{2}$ are displayed in figure 2.

4.2. *Critical curves for the square-well potential with spin–orbit interaction*

The second example deals with

$$V_1(r) = \Theta(R - r). \tag{44}$$

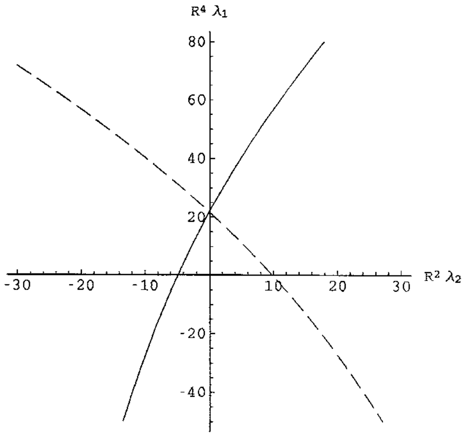

Figure 1. Critical curves for the states $\ell = 1$, $j = \frac{1}{2}$ (full curve) and $\ell = 1$, $j = \frac{3}{2}$ (broken curve) of the truncated harmonic potential with spin–orbit coupling are determined using JFM. The roots of $\mathcal{P}_5^{(1)}(\boldsymbol{\lambda})$ and $\mathcal{P}_6^{(1)}(\boldsymbol{\lambda})$ are indistinguishable in this figure.

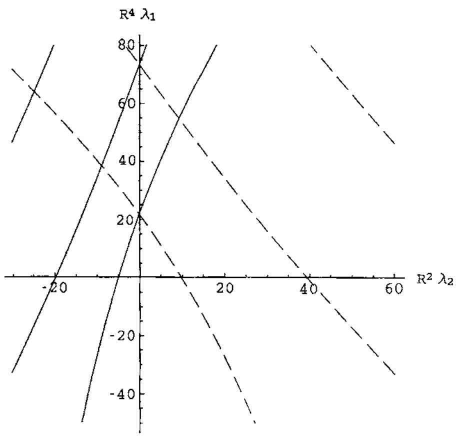

Figure 2. Critical curves for bound states with principal quantum number $n = 0$, 1 and 2 for $\ell = 1$, $j = \frac{1}{2}$ (full curve) and $\ell = 1$, $j = \frac{3}{2}$ (broken curve) of the truncated harmonic potential with spin–orbit coupling. They are determined from equation (B12).

The approximations to the critical curve, are obtained in the same way as for the preceding case. The results are plotted in figure 3 for $\ell = 1$, $j = \frac{1}{2}$ and $\ell = 1$, $j = \frac{3}{2}$. Again use has been made of the polynomials $\mathcal{P}_5^{(1)}(\boldsymbol{\lambda})$ and $\mathcal{P}_6^{(1)}(\boldsymbol{\lambda})$. Here, the two limits are distinguishable, contrary to the truncated harmonic case. Moreover, they are distinguishable in the region where the inequalities (38) are not satisfied.

Nevertheless, the differences are small, and the curves are very close to the corresponding exact solutions displayed in figure 4. Consequently, we reach the same conclusions as in the previous example: lower and upper boundaries give an excellent estimate of the critical curve in the parameter space where inequalities (38) are valid. The roots of $\mathcal{P}_6^{(1)}(\boldsymbol{\lambda})$, on the other hand, provide us with a fair approximation to the critical curve over the entire investigated parameter space.

For the sake of comparison, in figure 4 we give also the critical curves for the $n = 0$, 1 and 2 states. It is interesting to note from these curves that the limit $\lambda_1 = 0$ clearly shows that the shell-delta potential has no bound state for $n, \ell \neq 0$—a well known property of this potential.

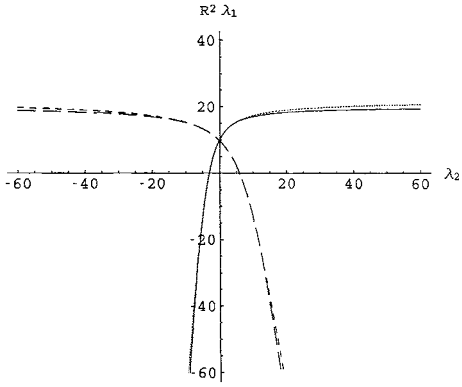

Figure 3. Critical curves for the states $\ell = 1$, $j = \frac{1}{2}$ (dotted and full curves) and $\ell = 1$, $j = \frac{3}{2}$ (broken curves, – – – and ———) of the square-well potential with spin–orbit coupling determined using JFM. The roots of $\mathcal{P}_5^{(1)}(\boldsymbol{\lambda})$ (dotted and short-broken curves) and $\mathcal{P}_6^{(1)}(\boldsymbol{\lambda})$ (full and long-broken curves) are distinguishable. Note that the roots of $\mathcal{P}_6^{(1)}(\boldsymbol{\lambda})$ are in good agreement with the exact values.

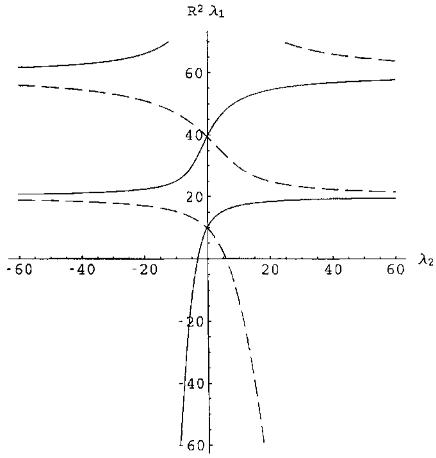

Figure 4. Critical curves for bound states with principal quantum number $n = 0, 1$ and 2 for $\ell = 1$, $j = \frac{1}{2}$ (full curve) and $\ell = 1$, $j = \frac{3}{2}$ (broken curve) of the square-well potential with spin–orbit coupling. They are determined from equation (B23).

5. Conclusions

This paper is devoted to the determination of the critical domain of coupling constants in multiple-component potentials of the form $U(r; \boldsymbol{\lambda}) = -\sum_{i=1}^{N} \lambda_i V_i(r)$. The positivity and the spherical symmetry of $V_i(r)$ are assumed. We also impose on $V_i(r)$ the usual conditions ensuring these components to be of short range and regular. Two general procedures have been proposed, which generalize methods used to handle the single-component case [2, 3]. One of these procedures has been used in conjunction with the JFM to treat multi-parameter critical domains.

For two-component potentials, explicit examples have been investigated: the truncated harmonic potential and the square-well potential, both with a spin–orbit part of the Thomas form. In the N-dimensional parameter space, the critical domain is given by an $(N-1)$-dimensional surface delimiting the regions with and without a bound state. It reduces to critical curves in the two-component case.

The present method has been applied to the two potentials mentioned above, by using polynomials of order five and six. While computing the critical curves, two situations are faced. If the inequalities (38) are satisfied, the roots of the polynomial $\mathcal{P}_5^{(1)}(\boldsymbol{\lambda})$ and $\mathcal{P}_6^{(1)}(\boldsymbol{\lambda})$ yield lower and upper boundaries, respectively. In the case when equation (38) is not satisfied, the roots are found to be close to each other, and those of $\mathcal{P}_6^{(1)}(\boldsymbol{\lambda})$ provide us with an accurate approximation. Generally, in regions where the boundaries exist, the present conclusions are safely extended to other potentials and higher parameter spaces. In regions where the inequalities (38) are not satisfied, we take as a conjecture that the roots of $\mathcal{P}_m^{(\ell)}(\boldsymbol{\lambda})$ approximate the critical curve (surface) with increasing accuracy as m increases.

The advantage of the chosen illustrative examples lies in the fact that they admit analytical solutions. Consequently, the approximate boundaries can be checked against exact values. A very satisfactory agreement has been found in these two cases.

Appendix A. Proof of the theorem stated in section 3

We assume that $V(r) \geqslant 0$ for $\forall r$ and $\lim_{r\to 0} r^2 V(r) = 0$. As was shown in [3], the coefficients a_j satisfy $a_j > 0$ and $a_{j+1}/a_j \leqslant M/2$. The series $R_{m+1}(\lambda)$ and polynomial $P_m(\lambda)$ are defined in equations (25) and (26).

We shall prove the following theorem by mathematical induction.

Theorem. *Provided $M^2 - 4a_2 \geqslant 0$, $\forall k \geqslant 2$, there exist the real zeros of polynomials $P_{2k-3}(\lambda)$, $P_{2k-2}(\lambda)$, $P_{2k-1}(\lambda)$, $P_{2k}(\lambda)$, denoted respectively by λ_{2k-3}, λ_{2k-2}, λ_{2k-1}, λ_{2k} and the real root λ_c of equation (22) so that the following series of inequalities is satisfied:*

$$\frac{1}{M} \leqslant \lambda_{2k-3} \leqslant \lambda_{2k-1} \leqslant \lambda_c \leqslant \lambda_{2k} \leqslant \lambda_{2k-2} \leqslant \frac{2}{M}. \tag{A1 = (29)}$$

Proof. The existence of real λ_c was proved in [3] as follows:

$$\varphi_0(r=0;\lambda_1) = P_1(\lambda_1) + R_2(\lambda_1) = R_2(\lambda_1) \geqslant 0 \tag{A2}$$

because λ_1 is the root of $P_1(\lambda)$. Provided $M^2 - 4a_2 \geqslant 0$, the root λ_2 of $P_2(\lambda)$ satisfies $\lambda_2 \leqslant 2/M$. Then,

$$\varphi_0(r=0;\lambda_2 \leqslant 2/M) = P_2(\lambda_2) + R_3(\lambda_2) = R_3(\lambda_2) \leqslant 0. \tag{A3}$$

Since $\varphi_0(r=0;\lambda)$ changes sign in the interval $(\lambda_1 = 1/M, \lambda_2)$, it has to exist a real root λ_c which satisfies

$$\frac{1}{M} = \lambda_1 \leqslant \lambda_c \leqslant \lambda_2 \leqslant \frac{2}{M}. \tag{A4}$$

From the uniqueness of λ_c and relations (A2)–(A4) it follows

$$\varphi_0(r=0;\lambda < \lambda_c) > 0 \tag{A5}$$

$$\varphi_0(r=0;\lambda_c < \lambda < 2/M) < 0. \tag{A6}$$

For $k = 2$ inequality (29) becomes the inequality (28), which was proved in [3] too. Let us now assume that the following inequality is satisfied:

$$\lambda_{2k-3} \leqslant \lambda_c \leqslant \lambda_{2k-2} \qquad k > 2. \tag{A7}$$

For $2/M \geqslant \lambda \geqslant 0$ the remainder $R_{2k+1}(\lambda) \leqslant 0$, so that it has to be $P_{2k}(\lambda_c) \geqslant 0$, in order that $\varphi_0(r=0;\lambda_c) = 0$ would be satisfied. We also have

$$P_{2k}(\lambda_{2k-2}) = P_{2k-2}(\lambda_{2k-2}) - a_{2k-1}\lambda_{2k-2}^{2k-1} + a_{2k}\lambda_{2k-2}^{2k} \leqslant 0 \tag{A8}$$

because λ_{2k-2} is a zero of the polynomial $P_{2k-2}(\lambda)$. This means that the polynomial $P_{2k}(\lambda)$ changes sign on the interval $[\lambda_c, \lambda_{2k-2}]$, so that there must exist the zero of the polynomial $P_{2k}(\lambda)$, denoted by λ_{2k}, such that $\lambda_c \leqslant \lambda_{2k} \leqslant \lambda_{2k-2}$.

The left-hand side of inequality (A1 = (29)) is proved in the same way. $P_{2k-1}(\lambda_c) \leqslant 0$, because $R_{2k}(\lambda) \geqslant 0$ for $2/M \geqslant \lambda \geqslant 0$. We also have

$$P_{2k-1}(\lambda_{2k-3}) = P_{2k-3}(\lambda_{2k-3}) + a_{2k-2}\lambda_{2k-3}^{2k-2} - a_{2k-1}\lambda_{2k-3}^{2k-1} \geqslant 0. \tag{A9}$$

The polynomial $P_{2k-1}(\lambda)$ changes sign on the interval $[\lambda_{2k-3}, \lambda_c]$, so that there must exist the zero of the polynomial $P_{2k-1}(\lambda)$, such that

$$\lambda_{2k-3} \leqslant \lambda_{2k-1} \leqslant \lambda_c. \tag{A10}$$

So, the left-hand side of the inequality (A1) is proved too. □

It is important to note that from relation (A5) and $R_{2k+1}(\lambda < 2/M) \leqslant 0$ it follows that $P_{2k}(\lambda < \lambda_c) > 0$. This means that $P_{2k}(\lambda)$ has no roots which are smaller than λ_c. Therefore, if there exists more than one real zero of polynomial $P_{2k}(\lambda)$ which are smaller than λ_2, the smallest among them is the best approximation for λ_c and should be taken for λ_{2k}.

Similarly, from the relation (A6) and $R_{2k}(\lambda < 2/M) \geqslant 0$ it follows that $P_{2k-1}(\lambda_c < \lambda < 2/M) < 0$. This means that $P_{2k-1}(\lambda)$ has no roots in the interval $(\lambda_c, 2/M)$. Therefore, if there exist more than one real zero of the polynomial $P_{2k-1}(\lambda)$ in the interval $(1/M, 2/M)$, the largest one should be taken in applying the inequality (29) for the determination of λ_c.

Appendix B. Exact solutions and critical curves for the two potentials of section 4

The first case is the truncated harmonic oscillator with spin–orbit potential

$$U(r;\boldsymbol{\lambda}) = -\lambda_1 V_1(r) + \lambda_2 \frac{1}{r}\frac{\partial V_1(r)}{\partial r}\vec{\ell}\cdot\vec{s} \tag{B1 = (42)}$$

with

$$V_1(r) = (R^2 - r^2)\Theta(R-r). \tag{B2}$$

The radial part of the corresponding Schrödinger equation for $s = \frac{1}{2}$ ($\hbar = 2m = 1$) is

$$\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\ell(\ell+1)}{r^2} - \lambda_1(R^2-r^2)\Theta(R-r) \right.$$
$$\left. -\lambda_2\Theta(R-r)\big(j(j+1) - \ell(\ell+1) - \tfrac{3}{4}\big) - E\right]\psi_{\ell j}(r) = 0. \tag{B3}$$

After the introduction of a new variable $x = r/R$, and taking $E = 0$, the latter equation takes the form

$$\left[-\frac{1}{x^2}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^2\frac{\mathrm{d}}{\mathrm{d}x}\right) + \frac{\ell(\ell+1)}{x^2} - \lambda_1' V_1'(x) - \lambda_2' V_2'(x)\right]\psi_{\ell j}(x) = 0. \tag{B4}$$

This is the radial part of the Schrödinger equation (for $E = 0$) with the effective potential

$$U'(x;\boldsymbol{\lambda}') = -\lambda_1' V_1'(x) - \lambda_2' V_2'(x) \tag{B5}$$

where

$$\begin{aligned} V_1'(x) &= (1-x^2)\Theta(1-x) \qquad & V_2'(x) &= \Theta(1-x) \\ \lambda_1' &= \lambda_{1c}R^4 & \lambda_2' &= \lambda_{2c}R^2\big(j(j+1) - \ell(\ell+1) - \tfrac{3}{4}\big). \end{aligned} \tag{B6}$$

The solution of equation (B4), which is proportional to x^ℓ near $x = 0$, is

$$\psi_{\ell j}(x) = \text{constant} \times \mathrm{e}^{-\sqrt{\lambda_1'}x^2/2}\big(\sqrt{\lambda_1'}x^2\big)^{\ell/2}\, {}_1F_1\left(\frac{\ell}{2} + \frac{3}{4} - \frac{\lambda_1' + \lambda_2'}{4\sqrt{\lambda_1'}}, \ell + \frac{3}{2}, \sqrt{\lambda_1'}x^2\right) \tag{B7}$$

where ${}_1F_1(a, b, x)$ is the confluent hypergeometric function. The logarithmic derivative $L(1-)$ of $\psi_{\ell j}(x)$ at $x = 1-$ is

$$L(1-) = \ell - \sqrt{\lambda_1'} + \left[2\sqrt{\lambda_1'}\left(\frac{\ell}{2} + \frac{3}{4} - \frac{\lambda_1' + \lambda_2'}{4\sqrt{\lambda_1'}}\right) {}_1F_1\left(\frac{\ell}{2} + \frac{7}{4} - \frac{\lambda_1' + \lambda_2'}{4\sqrt{\lambda_1'}}, \ell + \frac{5}{2}, \sqrt{\lambda_1'}\right)\right] \times\left[\left(\ell + \tfrac{3}{2}\right) {}_1F_1\left(\frac{\ell}{2} + \frac{3}{4} - \frac{\lambda_1' + \lambda_2'}{4\sqrt{\lambda_1'}}, \ell + \frac{3}{2}, \sqrt{\lambda_1'}\right)\right]^{-1}. \tag{B8}$$

In the region $x > 1$ we look for the solution of the equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{2}{x}\frac{\mathrm{d}}{\mathrm{d}x} + \frac{\ell(\ell + 1)}{x^2}\right]\psi_{\ell j} = 0. \tag{B9}$$

Imposing the required conditions, it reads

$$\psi_{\ell j}(x) = \text{constant} \times x^{-(\ell+1)}. \tag{B10}$$

The logarithmic derivative of the latter function at $x = 1+$ is

$$L(1+) = -(\ell + 1). \tag{B11}$$

The left and right logarithmic derivative at $x = 1$ have to be equated. This condition yields the following relation:

$$2\ell + 1 - \sqrt{\lambda_1'} + \left[2\sqrt{\lambda_1'}\left(\frac{\ell}{2} + \frac{3}{4} - \frac{\lambda_1' + \lambda_2'}{4\sqrt{\lambda_1'}}\right) {}_1F_1\left(\frac{\ell}{2} + \frac{7}{4} - \frac{\lambda_1' + \lambda_2'}{4\sqrt{\lambda_1'}}, \ell + \frac{5}{2}, \sqrt{\lambda_1'}\right)\right] \times\left[\left(\ell + \tfrac{3}{2}\right) {}_1F_1\left(\frac{\ell}{2} + \frac{3}{4} - \frac{\lambda_1' + \lambda_2'}{4\sqrt{\lambda_1'}}, \ell + \frac{3}{2}, \sqrt{\lambda_1'}\right)\right]^{-1} = 0. \tag{B12}$$

The values of parameters λ_1' and λ_2' which satisfy this equation determine critical pairs $(\lambda_{2c}R^2, \lambda_{1c}R^4)$.

The second case is the square-well potential with spin–orbit interaction:

$$U(r, \boldsymbol{\lambda}) = -\lambda_1\Theta(R - r) - \lambda_2\frac{1}{R}\delta(R - r)\vec{\ell}\cdot\vec{s}. \tag{B13}$$

The radial part of the corresponding Schrödinger equation ($\hbar = 2m = 1$) for $E = 0$ and $s = \frac{1}{2}$ is

$$\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\ell(\ell + 1)}{r^2} - \lambda_1\Theta(R - r) - \frac{\lambda_2}{R}\delta(R - r)\tfrac{1}{2}\left(j(j + 1) - \ell(\ell + 1) - \tfrac{3}{4}\right)\right]\psi_{\ell j}(r) = 0. \tag{B14}$$

After the transformation $\psi_{\ell j} = u_{\ell j}/r$ and the introduction of a new variable $x = r/R$, the latter equation takes the form

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\ell(\ell + 1)}{x^2} - \lambda_1'V_1'(x) - \lambda_2'V_2'(x)\right]u_{\ell j}(x) = 0 \tag{B15}$$

where

$$\begin{aligned} &U'(x, \boldsymbol{\lambda}') = -\lambda_1'V_1'(x) - \lambda_2'V_2'(x) \\ &V_1'(x) = \Theta(1 - x) \qquad V_2'(x) = \delta(1 - x) \\ &\lambda_1' = \lambda_{1c}R^2 \qquad \lambda_2' = \lambda_{2c}\tfrac{1}{2}\left(j(j + 1) - \ell(\ell + 1) - \tfrac{3}{4}\right). \end{aligned} \tag{B16}$$

By integrating equation (B15) from $1 - \xi$ to $1 + \xi$, where ξ is a small number, and by determining the limiting value of this integral when $\xi \to 0$, we obtain the condition

$$L(1+) - L(1-) + \lambda_2' = 0 \tag{B17}$$

where $L(1-)$ and $L(1+)$ are left and right logarithmic derivatives at $x = 1$.

If $\lambda_1' > 0$, the solution of equation (B15) which is proportional to $x^{\ell+1}$ near $x = 0$ is

$$u_{\ell j}(x) = \text{constant} \times x^{1/2} J_{\ell+1/2}\big(x/\sqrt{\lambda_1'}\big) \tag{B18}$$

where $J_{\ell+1/2}$ is the Bessel function. The logarithmic derivative $L(1-)$ for $\ell = 1$ is

$$L(1-) = \frac{\lambda_1' - 1 + \sqrt{\lambda_1'} \cot \sqrt{\lambda_1'}}{1 - \sqrt{\lambda_1'} \cot \sqrt{\lambda_1'}}. \tag{B19}$$

For $\lambda_1' < 0$ and $\ell = 1$ we find

$$L(1-) = \frac{-|\lambda_1'| - 1 + \sqrt{|\lambda_1'|} \coth \sqrt{|\lambda_1'|}}{1 - \sqrt{|\lambda_1'|} \coth \sqrt{|\lambda_1'|}}. \tag{B20}$$

In the region $x > 1$ we look for the solution of the equation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\ell(\ell+1)}{x^2}\right) u_{\ell j} = 0. \tag{B21}$$

Its solution, which does not diverge when $x \to \infty$, is

$$u_{\ell j} = \text{constant} \times x^{-\ell}$$

so that

$$L(1+) = -\ell. \tag{B22}$$

By substituting (B19), (B20) and (B22) into the condition (B17), for $\ell = 1$ we find

$$\lambda_2' = \begin{cases} \dfrac{\lambda_1' - 1 + \sqrt{\lambda_1'} \cot \sqrt{\lambda_1'}}{1 - \sqrt{\lambda_1'} \cot \sqrt{\lambda_1'}} + 1 & \lambda_1' > 0 \\[2ex] \dfrac{-|\lambda_1'| - 1 + \sqrt{|\lambda_1'|} \coth \sqrt{|\lambda_1'|}}{1 - \sqrt{|\lambda_1'|} \coth \sqrt{|\lambda_1'|}} + 1 & \lambda_1' < 0. \end{cases} \tag{B23}$$

References

[1] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (Oxford: Pergamon)

[2] Apenko S M 1983 Appearance of a bound state in the two-body problem and the ϵ expansion *Sov. Phys.–JETP Lett.* **38** 157

[3] Lassaut M and Lombard R J 1997 A sufficient condition for the existence of bound states for scalar spherically symmetric potentials *J. Phys. A: Math. Gen.* **30** 2467

[4] Lassaut M, Bulboaca S I and Lombard R J 1996 Critical behaviour of weakly bound systems *J. Phys. A: Math. Gen.* **29** 2175

[5] Apenko S M 1998 Weakly bound states in $2 + \epsilon$ dimensions *J. Phys. A: Math. Gen.* **31** 1553

[6] Newton R G 1982 *Scattering Theory of Waves and Particles* 2nd edn (New York: Springer)

[7] Hellmann G 1937 *Einführung in die Quantenchemie* (Leipzig)

[8] Feynman R P 1939 *Phys. Rev.* **56** 340