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'Critical' behaviour of weakly bound systems

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Abstract. We consider the class of three-dimensional finite-range, or similar, potentials $\lambda W(r)$, depending on a strength constant λ. We study the behaviour of the eigenvalue E as a function of $\lambda - \lambda_c$, where λ_c is the critical value at the transition from $0 \to 1$ bound state. For the $\ell = 0$ case, we find $E \propto (\lambda - \lambda_c)^2$, whereas the relationship is linear for $\ell \geqslant 1$. Treating ℓ as a continuous parameter in the radial Schrödinger equation, we give the evolution of the power law between $\ell = 0$ and $\ell = 1$. Besides spherically symmetric scalar potentials, we also discuss the case of a repulsive scalar potential combined with a spin–orbit component of the Thomas form.

1. Introduction

In a previous work [1], we have studied single neutron halo nuclei, characterized by a single neutron separation energy S_n which is very small, currently an order of magnitude lower than the average binding energy per particle $B(A)/A$. This is justifying a two-body approximation, and it has given us the motivation to discuss weakly bound states. In particular, we have found by means of a few numerical examples that the eigenvalue follows a power law in $\lambda - \lambda_c$ in the vicinity of λ_c, which is the critical value delimiting the transition between the zero and one bound state.

It is the purpose of the present paper to place this result on mathematical grounds. This problem is not restricted to nuclear physics but is encountered in any physical system of a weakly bound particle at the transition between zero and a few bound states. It should be the case of an electron weakly bound to a neutral atom, possibly in the presence of a magnetic field. Our results may also find an application in quantum wires, a subject of current interest [2, 3]. Finally, similar situations are found in field theory, when looking for possible bound states according to the values of the Lagrangian parameters [4].

Here we investigate finite-range or similar potentials $\lambda W(r)$ in three-dimensional space, depending on the strength constant λ. We consider first spherically symmetric scalar potentials. We find the power law to be quadratic for $\ell = 0$ states and linear for $\ell \geqslant 1$. The transition between these two cases is discussed by considering ℓ as a continuous parameter in the radial Schrödinger equation.

Note that the case of $\ell = 0$ states can be inferred from the potentials for which the analytical solution is well known, such as the Hulthén or the Morse potentials. The question is more delicate for the case of $\ell \geqslant 1$.

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Furthermore, we also discuss the case of a fixed repulsive scalar potential combined to a spin–orbit interaction of the Thomas form. We consider only the case of a spin-1/2 particle.

The paper is organized as follows. In section 2 the behaviour of the eigenvalues in the vicinity of λ_c is studied for scalar potentials. The case with a spin–orbit potential is discussed in section 3. Conclusions are drawn in section 4.

2. Scalar potential

In this section, we consider spherically symmetric scalar potentials $\lambda W(r)$ having at the most a finite number of bound states for a finite value of the strength constant λ. This class refer to finite-range potentials or to potentials decreasing fast enough to become negligible beyond a finite radius.

The Schrödinger equation reads

$$\left(-\frac{\hbar^2}{2m}\triangle + \lambda W(r)\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}). \tag{1}$$

Here, m is the mass of the single particle experiencing the potential W(r), and $\psi(\boldsymbol{r})$ the single particle wavefunction.

The usual decomposition on the spherical harmonics

$$\psi(\boldsymbol{r}) = \sum_{\ell,m} \frac{f_l(r)}{r} Y_\ell^m(\Omega) \tag{2}$$

eliminates the angular variables. We are left with the radial second-order differential equations depending on the value of the angular momentum ℓ,

$$f_\ell''(\lambda, E, r) = \left(\frac{2m}{\hbar^2}(-E + \lambda W(r)) + \frac{\ell(\ell+1)}{r^2}\right) f_\ell(\lambda, E, r) \tag{3}$$

where the prime denotes the derivatives with respect to the variable r.

Since $W(r)$ is assumed to decrease faster than $1/r^2$ at infinity, the Bargmann inequality [5] applies and gives us an upper bound for the number of bound states n_ℓ of the potential, involving only the attractive part W^+ of $W(r)$

$$n_\ell \leqslant -\frac{1}{2\ell+1}\frac{2m}{\hbar^2}\lambda \int_0^{+\infty} r W^+(r)\,\mathrm{d}r. \tag{4}$$

No bound state exists for $\lambda = 0$. For a sufficiently large value of λ, equation (4) at least suggests the occurrence of one bound state. For a large class of potentials, this is a sound conjecture, which can be put on firmer grounds, as shown in appendix A. It is obvious that the present work deals with potentials belonging to this class, and thus admitting at least one bound state for a large enough λ.

Although it can be intuitively inferred that λ_c corresponds to $E = 0$, it can be shown to be legitimate. The argument is quite general. Indeed, take the radial Schrödinger equation (3) having a bound state $E < 0$, for an attractive potential $\lambda W(r)$, and no bound state below λ_c. The function $f_\ell(\lambda, E, r)$ has the usual characteristics of bound state wavefunctions for the three-dimensional case: it vanishes at the origin and it is normalizable. When λ and E are varied simultaneously in a way to preserve the bound state, we have

$$\begin{aligned} f_\ell''(\lambda + \mathrm{d}\lambda, E + \mathrm{d}E, r) = {} & \left(\frac{2m}{\hbar^2}(-E - \mathrm{d}E + \lambda W(r) + \mathrm{d}\lambda W(r)) + l(l+1)/r^2\right) \\ & \times f_\ell(\lambda + \mathrm{d}\lambda, E + \mathrm{d}E, r). \end{aligned} \tag{5}$$

From the usual techniques and taking into account the boundary conditions for f_ℓ, we get

$$\frac{\mathrm{d}|E|}{\mathrm{d}\lambda} = -\int_0^{+\infty} W(r) f_\ell^2(\lambda, E, r)\,\mathrm{d}r \Bigg/ \int_0^{+\infty} f_\ell^2(\lambda, E, r)\,\mathrm{d}r. \tag{6}$$

In the case where $W(r)$ is negative, the right-hand side is positive definite, and therefore $|E|$ is an increasing continuous function of the variable λ. Reciprocally, λ is an increasing continuous function of $|E|$. Thus, the limiting value $E = 0$ provides us with the required 'critical' value λ_c.

Note that the same conclusion can be reached from the scattering state around $E = 0$. Indeed let $r(\lambda, E)$ be the first node of the Schrödinger equation for scattering states, equation (3) for $E > 0$. Remembering that $f_\ell(\lambda, E, r(\lambda, E))$ is identically zero and using the same technique as for (6), developed in [6], it is easy to show that

$$\frac{\partial r(\lambda, E)}{\partial E} = -\frac{2m}{\hbar^2} \frac{\int_0^{r(\lambda,E)} f_\ell^2(\lambda, E, r)\,\mathrm{d}r}{f_\ell'(\lambda, E, r(\lambda, E))^2}.$$

Accordingly, $E \mapsto r(\lambda, E)$ decreases when E increases. This function is monotonic; it can be inverted and the reciprocal $r \mapsto E(\lambda, r)$ can be defined. When the variable r tends to infinity, E either tends to zero or to a negative value corresponding to a bound state (see [6]). As E is continuous with respect to the parameter λ, the separation value λ_c between zero and one bound state corresponds to $E(\lambda_c, +\infty) = 0$. Therefore the energy corresponding to the transition is zero.

Equation (6) allows us to determine the behaviour of the energy $-E = |E|$ around the 'critical' value λ_c for values of the angular momentum $\ell > 1$. The function $f_\ell(\lambda_c, 0, r)$, corresponding to the transition towards a bound state, has asymptotic behaviour at infinity [5]:

$$\lim_{r\to+\infty} r^l f_\ell(\lambda_c, 0, r) = D \qquad D \neq 0.$$

For values of $\ell \geqslant 1$, $f_\ell(\lambda_c, 0, r)$ is therefore square integrable. From (6) we deduce the behaviour of the bound-state energy, E, at the vicinity of λ_c,

$$-E = \beta(\lambda - \lambda_c) \qquad \ell \geqslant 1 \tag{7}$$

where

$$\beta = -\int_0^{+\infty} W(r) f_\ell^2(\lambda_c, 0, r)\,\mathrm{d}r \Bigg/ \int_0^{+\infty} f_\ell^2(\lambda_c, 0, r)\,\mathrm{d}r. \tag{8}$$

For $\ell \geqslant 1$ the bound-state energy varies linearly with the energy.

The s-wave case is more delicate to discuss, since the function $f_0(\lambda_c, 0, r)$ becomes a constant at infinity. On the other hand, a number of analytically solvable models exist for this case, such as the Hulthén and the Morse potentials. They tell us that the energy variation obeys a quadratic law around the critical value

$$E \propto (\lambda - \lambda_c)^2.$$

The basic difference between s- and $\ell \geqslant 1$-waves is linked to the asymptotic behaviours of the wavefunctions. To demonstrate this statement, it is useful to consider the angular momentum ℓ as a continuous parameter in the radial Schrödinger equation. This procedure shows how the transition is occurring.

Let us stress again that $W(r)$ is supposed to become negligible beyond $r = R$. The method follows a reasoning valid for the square well potential. It estimates the logarithmic derivative at $r = R$:

$$v_\ell(\lambda, E, R) = f_\ell'(\lambda, E, R)/f_\ell(\lambda, E, R).$$

The value of R can be chosen arbitrarily since the final result does not depend crucially on it, as we shall see.

The asymptotic part of f_ℓ for continuous ℓ can be represented by

$$f_\ell(x) \propto q_\ell(x) = K_{\ell+1/2}(x)\sqrt{2x/\pi} \qquad x = \sqrt{-2m/\hbar^2 E}R$$

where the function K_ν is the modified Bessel function of the third kind [7, 8].

In order to discuss v_ℓ around $E = 0$, we need the ascending series expansion of q_ℓ in the power of x. This is given by

$$q_\ell(x) = \frac{\sqrt{\pi}}{\cos(\ell\pi)} \frac{2^\ell}{x^\ell} \left(\sum_{n=0}^{+\infty} \frac{(x/2)^{2n}}{n!\Gamma(n-\ell+1/2)} - \sum_{n=0}^{+\infty} \frac{(x/2)^{2n+2\ell+1}}{n!\Gamma(n+l+3/2)} \right) \tag{9}$$

which can also be written as

$$q_\ell(x) = \frac{\sqrt{\pi}}{\cos(\ell\pi)} \frac{2^\ell}{x^\ell} \left(- \sum_{n=0}^{n\leqslant \ell-1/2} \left(\frac{x}{2}\right)^{2n} \frac{\Gamma(\ell-n+1/2)}{n!} \frac{\sin(\pi(\ell-n-1/2))}{\pi} \right.$$
$$\left. + \sum_{n>\ell-1/2}^{+\infty} \frac{(x/2)^{2n}}{n!\Gamma(n-\ell+1/2)} - \sum_{n=0}^{+\infty} \frac{(x/2)^{2n+2\ell+1}}{n!\Gamma(n+l+3/2)} \right). \tag{10}$$

This expression is valid for every $(\ell - 1/2)$ not integer. In the latter case, the function $q_\ell(x)$ is defined by continuity. It is immediate to observe that the value $\ell = 1/2$ constitutes a boundary. Consequently, from the behaviour of $q_\ell(x)$ as E or equivalently x tends to zero, we distinguish three estimates of the logarithmic derivative, namely

$$v_\ell(\lambda, E, R) = -\frac{\ell}{R}\left(1 - \frac{2m}{\hbar^2}\frac{ER^2}{\ell(2\ell-1)}\right) \qquad \ell > 1/2 \tag{11}$$

$$v_\ell(\lambda, E, R) = -\frac{\ell}{R}\left(1 + \left(\frac{-mER^2}{2\hbar^2}\right)^{(2\ell+1)/2} \frac{2\pi}{\Gamma(\ell+1/2)^2\ell\cos(\pi\ell)}\right) \qquad \ell < 1/2 \tag{12}$$

and

$$v_\ell(\lambda, E, R) = -\frac{1}{2R}\left(1 + \frac{2m}{\hbar^2}R^2 E\ln(-E)\right) \qquad \ell = 1/2. \tag{13}$$

More details concerning these estimates are given in appendix B. Going back to the Schrödinger equation, we use the same procedure as before, varying λ and E in a way to preserve the bound state and get

$$f_\ell''(\lambda + \mathrm{d}\lambda, E + \mathrm{d}E, r) f_\ell(\lambda, E, r) - f_\ell''(\lambda, E, r) f_\ell(\lambda + \mathrm{d}\lambda, E + \mathrm{d}E, r)$$
$$= \frac{2m}{\hbar^2}(-\mathrm{d}E\, f_\ell(\lambda, E, r)^2 + \mathrm{d}\lambda\, W(r) f_\ell(\lambda, E, r)^2). \tag{14}$$

Neglecting second-order terms, $(\mathrm{d}E)^2$, $\mathrm{d}E\,\mathrm{d}\lambda$ and $\mathrm{d}\lambda^2$, this equation yields

$$f_\ell'(\lambda + \mathrm{d}\lambda, E + \mathrm{d}E, r) f_\ell(\lambda, E, r) - f_\ell'(\lambda, E, r) f_\ell(\lambda + \mathrm{d}\lambda, E + \mathrm{d}E, r)$$
$$= \frac{2m}{\hbar^2}\left(- \mathrm{d}E \int_0^r f_\ell(\lambda, E, r')^2\,\mathrm{d}r' + \mathrm{d}\lambda \int_0^r W(r') f_\ell(\lambda, E, r')^2\,\mathrm{d}r' \right). \tag{15}$$

Therefore,

$$\left(\frac{\partial^2 f_\ell}{\partial r \partial\lambda}(\lambda, E, r)\,\mathrm{d}\lambda + \frac{\partial^2 f_\ell}{\partial r \partial E}(\lambda, E, r)\,\mathrm{d}E\right) f_\ell(\lambda, E, r)$$
$$- \frac{\partial f_\ell}{\partial r}(\lambda, E, r)\left(\frac{\partial f_\ell}{\partial\lambda}(\lambda, E, r)\,\mathrm{d}\lambda + \frac{\partial f_\ell}{\partial E}(\lambda, E, r)\,\mathrm{d}E\right)$$
$$= \frac{2m}{\hbar^2}\left(- \mathrm{d}E \int_0^r f_\ell(\lambda, E, r')^2\,\mathrm{d}r' + \mathrm{d}\lambda \int_0^r W(r') f_\ell(\lambda, E, r')^2\,\mathrm{d}r' \right). \tag{16}$$

From this, provided that $f_\ell(\lambda, E, r) \neq 0$, the logarithmic derivative $v_\ell(\lambda, E, r)$ satisfies

$$\left(\frac{\partial v_\ell}{\partial\lambda}(\lambda, E, r)\,\mathrm{d}\lambda + \frac{\partial v_\ell}{\partial E}(\lambda, E, r)\,\mathrm{d}E\right) f_\ell(\lambda, E, r)^2$$
$$= \frac{2m}{\hbar^2}\left(-\,\mathrm{d}E\int_0^r f_\ell(\lambda, E, r')^2\,\mathrm{d}r' + \mathrm{d}\lambda\int_0^r W(r')f_\ell(\lambda, E, r')^2\,\mathrm{d}r'\right). \qquad (17)$$

On the other hand, in the vicinity of $E = 0$, $\lambda = \lambda_c$, $v_\ell(\lambda, E, R)$ admits a limited expansion

$$v_\ell(\lambda, E, R) \simeq v_\ell(\lambda_c, 0, R) + \frac{\partial v_\ell}{\partial\lambda}(\lambda_c, 0, R)(\lambda - \lambda_c) + \frac{\partial v_\ell}{\partial E}(\lambda_c, 0, R)E. \qquad (18)$$

According to (17) and (18), it follows that

$$\frac{2m}{\hbar^2}\left(-\,E\int_0^R f_\ell(\lambda_c, 0, r')^2\,\mathrm{d}r' + (\lambda - \lambda_c)\int_0^R W(r')f_\ell(\lambda_c, 0, r')^2\,\mathrm{d}r'\right)$$
$$= -\,\frac{\ell}{R}f_\ell^2(\lambda_c, 0, R)g(E)$$

where $g(E)$ is defined by $v_\ell(\lambda, E, R) = -(\ell/R)(1 + g(E))$. Taking into account equations (11) and (12), for $\ell \neq 1/2$, the two cases $g(E) \propto E$ $(\ell > 1/2)$ and $g(E) \propto E^{(2\ell+1)/2}$ $(\ell < 1/2)$ yield the following expressions,

$$-E = \beta(\lambda - \lambda_c) \qquad \ell > 1/2 \qquad (19)$$

with

$$\beta = -\int_0^R W(r')f_\ell^2(\lambda_c, 0, r')\,\mathrm{d}r' \Bigg/ \left(\int_0^R f_\ell^2(\lambda_c, 0, r')\,\mathrm{d}r' + \frac{R}{2\ell - 1}f_\ell^2(\lambda_c, 0, R)\right) \qquad (20)$$

and

$$-E = \beta(\lambda - \lambda_c)^{2/(2\ell+1)} \qquad \ell < 1/2 \qquad (21)$$

with

$$\beta = \frac{2\hbar^2}{mR^2}\left(-\frac{mR\cos(\pi\ell)\Gamma(\ell + 1/2)^2\int_0^R W(r')f_\ell^2(\lambda_c, 0, r')\,\mathrm{d}r'}{\pi\hbar^2 f_\ell(\lambda_c, 0, R)^2}\right)^{2/(2\ell+1)}. \qquad (22)$$

For $\ell = 1/2$ we have

$$-E = G\left((\lambda - \lambda_c)\frac{2}{R}\frac{\int_0^R W(r')f_\ell^2(\lambda_c, 0, r')\,\mathrm{d}r'}{f_\ell(\lambda_c, 0, R)^2}\right) \qquad (23)$$

where G denotes the reciprocal of the function $x\ln(x)$ taken at the vicinity of zero.

Although the derivation of the variation of the energy near λ_c uses arguments strictly valid for finite-range potentials, the generalization to any potential satisfying the usual integrability conditions ($W(r)$ and $rW(r)$ integrable) is easy to prove. Indeed, the above expression for β does not depend crucially on R. This is obvious for the integrals involving the potential, in which the upper limit can be set to infinity.

For the case $\ell > 1/2$, the term $Rf_\ell(\lambda_c, 0, R)$ tends to zero as $R^{2\ell-1}$, and the function f_ℓ is square integrable. Thus the limiting value of β is

$$\beta = -\int_0^{+\infty} W(r')f_\ell^2(\lambda_c, 0, r')\,\mathrm{d}r' \Bigg/ \int_0^{+\infty} f_\ell^2(\lambda_c, 0, r')\,\mathrm{d}r' \qquad (24)$$

identical to that of equation (8).

For the two other cases, because $f_\ell \propto \text{constant} \times r^{-\ell}$ for $r > R$, β becomes independent of R, except through the integral over the potential. More precisely

$$\beta = \frac{2\hbar^2}{m}\left(-\frac{m\cos(\pi\ell)\Gamma(\ell+1/2)^2}{\pi\hbar^2}\int_0^{+\infty} W(r')f_\ell^2(\lambda_c, 0, r')\,\mathrm{d}r'\right)^{2/(2\ell+1)} \qquad \ell < 1/2 \tag{25}$$

in particular, we recover a quadratic law for the $\ell = 0$ case, and

$$-E = G\left((\lambda-\lambda_c)2\int_0^R W(r')f_\ell^2(\lambda_c, 0, r')\,\mathrm{d}r'\right) \qquad \ell = 1/2 \tag{26}$$

where, in equations (25) and (26), $\lim_{r\to+\infty} r^\ell f_\ell(r)$ is chosen equal to unity.

These few remarks, together with the fact that the point R can always be chosen in a region where the asymptotic form of the wavefunction dominates, make our derivation valid for any potential having a finite number of bound states and becoming negligible beyond some point.

We shall conclude this section with two illustrative examples, for which the analytical solution is well known and can be found in many textbooks. Here we shall adopt the notation of Flügge [9].

For the Hulthén potential

$$V(r) = -V_0\frac{\mathrm{e}^{-r/a}}{1-\mathrm{e}^{-r/a}}$$

the eigenvalues are given by

$$E_n = -V_0\left(\frac{\beta^2-n^2}{2n\beta}\right)^2 \qquad \beta \geqslant n$$

for the s-wave with $\beta^2 = 2mV_0a^2/\hbar^2$.

The transition from the zero to one state (or the $n-1$ to n states) occurs for $V_0^c = \hbar^2/(2ma^2)$ (or $V_0^{c,n} = n^2\hbar^2/(2ma^2)$). As expected, in the vicinity of $V_0^{c,n}$ the eigenvalues E_n follow a quadratic law

$$E_n = -\frac{m}{2\hbar^2}\frac{a^2}{n^2}(V_0 - V_0^{c,n})^2.$$

The three-dimensional square well potential gives an opportunity to look for higher ℓ values. With the notation of [9], $V(r) = -V_0$; $r < R$ and zero outside, the lowest bound-state energy E_1 is the lowest solution of

$$\tan(x_0\xi) = f_\ell(x_0, \xi)$$

for the ℓ-wave, where $f_\ell(x_0,\xi)$ is given in [9], in terms of $x_0 = R\sqrt{2mV_0/\hbar^2}$ and $\xi = \sqrt{(V_0-|E|)/V_0}$. Here we study both cases $\ell = 0$ and $\ell = 1$. The corresponding values of $f_\ell(x_0,\xi)$ are, respectively,

$$f_0(x_0,\xi) = -\frac{\xi}{\sqrt{1-\xi^2}}$$

$$f_1(x_0,\xi) = \frac{x_0\xi(1-\xi^2)}{1-\xi^2+\xi^2(1+x_0\sqrt{1-\xi^2})}.$$

The transition from the zero to one bound state occurs for $\xi = 1$ therefore $x_0\xi$ is equal to either $\pi/2$ ($\ell = 0$) or π ($\ell = 1$). The variation of the eigenenergy E_1 in terms of $V_0 - V_0^c$ given by

$$|E_1| = \frac{m}{2\hbar^2}R^2(V_0 - V_0^c)^2 \qquad \ell = 0$$

and

$$|E_1| = \tfrac{1}{3}(V_0 - V_0^c) \qquad \ell = 1$$

follows quadratic and linear laws according to our previous statements.

3. Scalar plus spin–orbit potentials

It is interesting to perform the same kind of investigation in the case of a potential having a scalar and a spin–orbit component. We consider here only the case of a spin-1/2 particle. In fact the problem would be similar (if not simpler) for any vector potential coupled to the spin $\lambda \boldsymbol{W}(\boldsymbol{r}) \cdot \boldsymbol{s}$. In the present work we focus our attention on the spin–orbit interaction. Other cases may be developed in future work, if they are found to be of particular interest. We chose the scalar part to be strictly repulsive, so that bound states can only originate from the spin–orbit contribution. It can be parametrized in various ways. We choose here a Thomas form. The total potential is thus written

$$W(r) = U(r) - \frac{\lambda}{r}\frac{\partial}{\partial r}U(r)\boldsymbol{\ell} \cdot \boldsymbol{s}. \tag{27}$$

In the case of a repulsive central force, only the spin–orbit sublevels $j = \ell - 1/2$ have a chance to be bound, the $j = \ell + 1/2$ partners staying in the continuum. Thus we are left with ($\ell \geqslant 1$):

$$f_\ell''(\lambda, E, r) = \left(\frac{2m}{\hbar^2}(-E + U(r) + \frac{\lambda}{2}(\ell+1)\frac{1}{r}\frac{\partial}{\partial r}U(r)) + \frac{\ell(\ell+1)}{r^2}\right) f_\ell(\lambda, E, r). \tag{28}$$

The Bargmann inequality becomes

$$n_l \leqslant -\lambda \frac{m}{\hbar^2}\frac{\ell+1}{2\ell+1}\int_0^{+\infty} \frac{\partial}{\partial r}U(r)\,\mathrm{d}r.$$

Although the previous conclusions about the transition law around λ_c are still valid we investigate here a soluble model, namely the square well potential:

$$U(r) = U_0\Theta(R_0 - r). \tag{29}$$

The radial Schrödinger equation for this case reads

$$f_\ell''(\lambda, k, r) = \left(k^2 + \tilde{U}_0\Theta(R_0 - r) - \frac{\lambda}{2}\frac{(\ell+1)}{r}\tilde{U}_0\delta(r - R_0) + \frac{\ell(\ell+1)}{r^2}\right) f_\ell(\lambda, k, r) \tag{30}$$

where we have put $k^2 = -2mE/\hbar^2$, $\tilde{U}_0 = 2mU_0/\hbar^2$.

The δ distribution is known to produce a discontinuity in the derivative of the wavefunction at R_0. Assuming that $f_\ell(\lambda, k, r)$ is constant over an infinitesimal interval centred on R, the difference between the right and left logarithmic derivatives of the wavefunction is given by

$$\left.\frac{f_\ell'(\lambda, k, r)}{f_\ell(\lambda, k, r)}\right|_{\mathrm{R}} - \left.\frac{f_\ell'(\lambda, k, r)}{f_\ell(\lambda, k, r)}\right|_{\mathrm{L}} = -\frac{\lambda}{2R_0}(\ell+1)\tilde{U}_0.$$

The solutions of (30) for a bound state are given by

$$\begin{aligned} f_\ell(\lambda, k, r) &= x\tilde{j}_\ell(x) \qquad x = r\sqrt{k^2 + \tilde{U}_0} \qquad r \leqslant R_0 \\ f_\ell(\lambda, k, r) &= C(k)\mathrm{e}^{-kr}P_\ell(kr) \qquad r \geqslant R_0 \end{aligned} \tag{31}$$

where $C(k)$ is obtained from the continuity condition at $r = R_0$. Use is made here of the spherical modified Bessel function of the first kind $\tilde{j}_\ell(x) = \sqrt{\pi/(2x)}I_{\ell+1/2}(x)$, and of the polynomial $P_\ell(x)$ defining the asymptotic behaviour of the modified Hankel's first kind function $K_{\ell+1/2}(x)\sqrt{2x/\pi}$ (see Abramowitz and Stegun [7] or Erdélyi [8]):

$$P_\ell(kr) = \sum_{p=0}^{\ell} \frac{(l+p)!}{p!(l-p)!}(2kr)^{-p}. \tag{32}$$

It is straightforward to obtain the following equation for the logarithmic derivative at R_0:

$$\frac{\tilde{j}_\ell(x_0) + x_0 \tilde{j}_\ell(x_0)'_x}{\tilde{j}_\ell(x_0)} - \frac{\lambda}{2}\tilde{U}_0(\ell+1) = -kR_0 \frac{P_\ell(kR_0) - P'_\ell(kR_0)/k}{P_\ell(kR_0)} \tag{33}$$

where $x_0 = R_0\sqrt{k^2 + \tilde{U}_0}$. Here the symbol $'_x$ denotes the derivative with respect to x.

In the vicinity of $k = 0$, the right-hand side of (33) therefore reads

$$-l\left(1 + \frac{1}{l(2l-1)}k^2 R_0^2\right) \qquad \forall l \geqslant 1.$$

Similarly, the left-hand side of (33) reads $(k = 0, \lambda = \lambda_c)$

$$\frac{\tilde{j}_\ell(x_c) + x_c \tilde{j}_\ell(x_c)'_x}{\tilde{j}_\ell(x_c)} + (x_0 - x_c)\frac{-\tilde{j}_\ell(x_c)'_x \tilde{j}_\ell(x_c) + x_c(\tilde{j}_\ell^2(x_c) - \tilde{j}_\ell^2(x_c)'_x) + \ell(\ell+1)/x_c \tilde{j}_\ell^2(x_c)}{\tilde{j}_\ell^2(x_c)}$$
$$-\frac{\lambda_c}{2}(\ell+1)\tilde{U}_0 - \frac{\lambda - \lambda_c}{2}(\ell+1)\tilde{U}_0$$

where $x_c = R_0\sqrt{\tilde{U}_0}$. Since $(x_0 - x_c)$ varies with k^2, E is linearly dependent on $\lambda - \lambda_c$ as in the scalar case,

$$-E = \beta(\lambda - \lambda_c) \tag{34}$$

where

$$\beta = \frac{\hbar^2}{2m}\frac{(\ell+1)\tilde{U}_0^2 \tilde{j}_\ell^2(x_c)}{x_c^2(2\ell+1)\tilde{j}_\ell(x_c)^2/(2\ell-1) - (1+2\ell)x_c \tilde{j}_\ell(x_c)\tilde{j}_{\ell+1}(x_c) - x_c^2 \tilde{j}_{\ell+1}^2(x_c)}. \tag{35}$$

To get equation (35), use is made of the recurrence relation

$$\tilde{j}_\ell(x_c)'_x = \frac{\ell}{x_c}\tilde{j}_\ell(x_c) + \tilde{j}_{\ell+1}(x_c).$$

It should be noted that such a critical behaviour, obtained by expanding both sides of (33) around $k = 0$ and $\lambda = \lambda_c$, results from the fact that the linear term in k vanishes. As far as the Bessel function is concerned, since the argument depends on k according to $\sqrt{k^2 + \tilde{U}_0}$, the expansion of the left-hand side yields a term proportional to k^2.

For the spin–orbit potential, it is interesting to look for the behaviour of λ_c against ℓ. In the present model it is given by

$$\frac{\lambda_c}{2}(\ell+1)\tilde{U}_0 = (2\ell+1) + x_c\frac{\tilde{j}_{\ell+1}(x_c)}{\tilde{j}_\ell(x_c)}.$$

Since the $\tilde{j}_\ell(x_c)$ are positive definite, it shows that $\lambda_c \geqslant 2\tilde{U}_0^{-1}(2\ell+1)/(\ell+1)$, which gives for $\lambda_c(\ell)$ a lower limit increasing with ℓ. Exact values of $\lambda_c(\ell)$ are displayed in figure 1. For low values of x_c, $x_c \leqslant 1.8$, (remember that $x_c^2 = \tilde{U}_0 R_0^2 \propto \int_0^{+\infty} rU(r)\,\mathrm{d}r$), λ_c is an increasing function of ℓ. Beyond this 'empirical' value of 1.8, λ_c increases only for high enough values of ℓ. The regime is thus not unique. It is clearly shown that the most intuitive situation, in which λ_c is a continuously increasing function of ℓ, is not universal. Consequently, $\lambda_c(\ell)$ depends on the geometry of the potential.

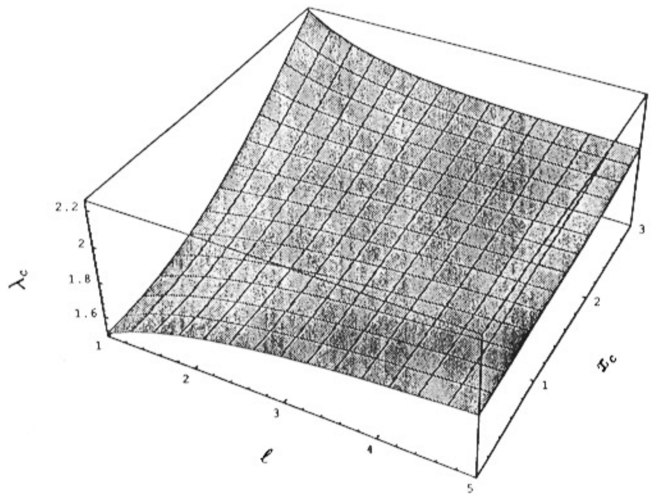

Figure 1. Critical value λ_c as a function of the orbital momentum ℓ and the parameter x_c, linked to the geometry of the potential (see text).

4. Conclusions

In the present work we have studied the variation of the energy eigenvalue E of a weakly bound particle in the vicinity of a critical value of the strength constant λ_c. For a potential $\lambda W(r)$ becoming negligible beyond a given radius, the critical value corresponds to the transition between the zero and one bound state.

For scalar, spherically symmetric potentials, E varies quadratically with $(\lambda - \lambda_c)$ around λ_c for the s-state. The variation is linear for $\ell \geqslant 1$. In fact, by letting ℓ to be a continuous parameter of the radial Schrödinger equation, we found that the evolution of the power law is continuous from $-1/2 \leqslant \ell \leqslant 1/2$.

Investigating the case of a spin–orbit potential, for a spin-1/2 particle combined with a scalar repulsive potential, we show that the energy E also follows a linear power law around λ_c, for the subspace of states with $j = \ell - 1/2$.

The present discussion was focused on the transition between the zero and one bound state. The same arguments can be used to investigate the transition between the $n - 1$ and n bound states. Since we are primarily interested in potentials with a finite number of bound states, n should not be too large. The basic arguments, however, are based on the asymptotic behaviour of the wavefunctions and, thus, are independent of the number of nodes. In particular the transition laws still hold.

Although it may have no application, it is also interesting to note that in the case of a scalar potential the ensemble of the critical values λ_n is univocally connected to the ensemble of the bound-state energies when the potential W, equation (3), is purely attractive and satisfies $\int_0^{+\infty} \sqrt{-W(r)}\, \mathrm{d}r < +\infty$. Indeed, if the critical values are known, they can be used to reconstruct the potential [5, 10].

Appendix A

We start from equation (3):

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} f_\ell(\lambda, E, r) = \left(\frac{2m}{\hbar^2}(-E + \lambda W(r)) + \frac{\ell(\ell+1)}{r^2}\right) f_\ell(\lambda, E, r). \tag{A1}$$

Following [5, 10], use is made of the Liouville transformation

$$r \mapsto Z(r) = \int_0^r \sqrt{-\frac{2m}{\hbar^2} W(r')}\, \mathrm{d}r'$$

$$f_\ell(\lambda, E, r) = \left(-\frac{2m}{\hbar^2} W(r)\right)^{-1/4} \psi_\ell(\lambda, E, Z).$$

Equation (A1) becomes

$$\frac{\mathrm{d}^2}{\mathrm{d}Z^2} \psi_\ell''(\lambda, E, Z) + (\lambda - q(Z))\psi_\ell(\lambda, E, Z) = 0 \tag{A2}$$

where

$$q(Z) = \frac{\hbar^2}{2m}\left(-\frac{W''_{r^2}}{4W^2}(r(Z)) + \frac{5}{16}\frac{W_r'^2}{W^3}(r(Z)) - \frac{\ell(\ell+1)}{r^2(Z)W(r(Z))}\right) + \frac{E}{W(r(Z))}. \tag{A3}$$

For the potentials we are considering in the present work, $Z \in [0, I]$ where $I = \int_0^{+\infty} \sqrt{-(2m/\hbar^2)W(r)}\, \mathrm{d}r < +\infty$. A bound state of energy $-E$ corresponds to $f_\ell(\lambda, E, 0) = f_\ell(\lambda, E, +\infty) = 0$ which is mapped into $\psi_\ell(\lambda, E, 0) = \psi_\ell(\lambda, E, I) = 0$.

For $\lambda = 0$, equation (A1) has no bound state. This means that fixing the boundary conditions at one extremity of the segment, say $\psi_\ell(0, E, 0) = 0$, we have automatically $\psi_\ell(0, E, I) \neq 0$. The strength parameter λ, however, is acting as a Lagrange multiplier, and can be chosen in a way to ensure $\psi_\ell(\lambda, E, I) = 0$ together with $\psi_\ell(\lambda, E, 0) = 0$. Note that E plays no major role; apart from being negative it can be chosen close to zero.

To show that the value of λ corresponding to a given energy $-E$ must be positive and finite, we multiply the Schrödinger equation (A1) by $f_\ell(\lambda, E, r)$ from the left and integrate. This yields

$$\frac{\hbar^2}{2m}\int_0^{+\infty} f_\ell'(\lambda, E, r)^2\, \mathrm{d}r - \lambda \int_0^{+\infty} |W(r)| f_\ell(\lambda, E, r)^2\, \mathrm{d}r + \frac{\hbar^2}{2m}\ell(\ell+1)\int_0^{+\infty} \frac{f_\ell(\lambda, E, r)^2}{r^2}\, \mathrm{d}r = E\int_0^{+\infty} f_\ell(\lambda, E, r)^2\, \mathrm{d}r.$$

The four integrals being positive definite, $E < 0$ requires $\lambda > 0$.

Finally, using the virial theorem [11], we have

$$\lambda\left(-\frac{3}{2}\int_0^{+\infty} f_\ell(\lambda, E, r)^2 r\left(\frac{\mathrm{d}}{\mathrm{d}r}|W(r)|\right) \mathrm{d}r - \int_0^{+\infty} |W(r)| f_\ell(\lambda, E, r)^2\, \mathrm{d}r\right) = E\int_0^{+\infty} f_\ell(\lambda, E, r)^2\, \mathrm{d}r. \tag{A4}$$

Because $E < 0$, we have

$$\int_0^{+\infty} |W(r)| f_\ell(\lambda, E, r)^2\, \mathrm{d}r > -\frac{3}{2}\int_0^{+\infty} f_\ell(\lambda, E, r)^2 r\left(\frac{\mathrm{d}}{\mathrm{d}r}|W(r)|\right) \mathrm{d}r.$$

For the class of potentials considered here, $\int_0^{+\infty} |W(r)| f_\ell(\lambda, E, r)^2\, \mathrm{d}r$ is finite and thus, from (A4), λ is finite.

Appendix B

The modified Bessel function of the third kind is defined by [8]

$$K_\nu(x) = \frac{\pi}{2\sin(\pi\nu)}(I_{-\nu}(x) - I_\nu(x))$$

in terms of the function I_ν. Remembering that we have defined $\tilde{j}_\ell(x)$ as $\tilde{j}_\ell(x) = \sqrt{\pi/(2x)}I_{\ell+1/2}(x)$ we have

$$q_\ell(x) = \frac{x}{\cos(\ell\pi)}(\tilde{j}_{-\ell-1}(x) - \tilde{j}_\ell(x)).$$

The present definition of $q_\ell(x)$ corresponds to the asymptotic behaviour $\lim_{x\to+\infty} q_\ell(x)\exp(x) = 1$. Taking into account

$$\tilde{j}_\ell(x) = \frac{\sqrt{\pi}}{2}\sum_{m=0}^{+\infty}\frac{(x/2)^{2m+\ell}}{m!\Gamma(m+\ell+3/2)}$$

we easily obtain for non-integer values of $\ell + 1/2$,

$$q_\ell(x) = \frac{\sqrt{\pi}}{\cos(\ell\pi)}\frac{2^\ell}{x^\ell}\left(\sum_{m=0}^{+\infty}\frac{(x/2)^{2m}}{m!\Gamma(m-\ell+1/2)} - \sum_{m=0}^{+\infty}\frac{(x/2)^{2m+2\ell+1}}{m!\Gamma(m+l+3/2)}\right). \tag{B1}$$

Using the properties of the Γ function it becomes

$$q_\ell(x) = \frac{\sqrt{\pi}}{\cos(\ell\pi)}\frac{2^\ell}{x^\ell}\left(-\sum_{m=0}^{m\leqslant\ell-1/2}\left(\frac{x}{2}\right)^{2m}\frac{\Gamma(\ell-m+1/2)}{m!}\frac{\sin(\pi(\ell-m-1/2))}{\pi}\right.$$
$$\left. + \sum_{m>\ell-1/2}^{+\infty}\frac{(x/2)^{2m}}{m!\Gamma(m-\ell+1/2)} - \sum_{m=0}^{+\infty}\frac{(x/2)^{2m+2\ell+1}}{m!\Gamma(m+l+3/2)}\right). \tag{B2}$$

The expression of q_ℓ for $\ell = n + 1/2, n \in \mathbb{N}$ is deduced from expression (B2) at the limit $\ell \to n + 1/2$,

$$q_{n+1/2}(x) = \frac{1}{\sqrt{\pi}}\left(\frac{2}{x}\right)^{n+1/2}\left(\sum_{m=0}^{n}(-)^m\left(\frac{x}{2}\right)^{2m}\frac{(n-m)!}{m!}\right.$$
$$\left. +(-)^{n+1}\sum_{m=0}^{+\infty}\left(\frac{x}{2}\right)^{2m+2n+2}\frac{\psi(n+m+2)+\psi(m+1)-2\ln(x/2)}{m!(n+m+1)!}\right) \tag{B3}$$

or equivalently remembering that $n = \ell - 1/2$,

$$q_\ell(x) = \frac{1}{\sqrt{\pi}}\left(\frac{2}{x}\right)^{\ell}\left(\sum_{m=0}^{\ell-1/2}(-)^m\left(\frac{x}{2}\right)^{2m}\frac{(\ell-m-1/2)!}{m!}\right.$$
$$\left. +(-)^{\ell+1/2}\sum_{m=0}^{+\infty}\left(\frac{x}{2}\right)^{2m+2\ell+1}\frac{\psi(\ell+m+3/2)+\psi(m+1)-2\ln(x/2)}{m!(\ell+m+1/2)!}\right). \tag{B4}$$

The transition law around $\lambda - \lambda_c$ requires the knowledge of the logarithmic derivative of $q_\ell(x)$ at the vicinity of zero. Equation (B1) incorporates two kinds of powers of the variable x: x^{2m} and $x^{2m+2\ell+1}$. We have $2m + 2\ell + 1 > 2$ ($\forall\ell > 1/2$), and the first appearing power of x is quadratic. For low values of x, we get

$$q_\ell(x) \propto 1 + ax^2.$$

For $\ell < 1/2$ the term in $x^{2\ell+1}$ dominates with respect to x^2 and we find

$$q_\ell(x) \propto 1 + ax^{2\ell+1}.$$

The logarithmic derivative of q_ℓ then satisfies (11) and (12). For $\ell = 1/2$ use is made of (B4) where the dominant term, besides the constant, behaves like $x^2 \ln(x) \simeq x^2 \ln(x^2)$.

References

[1] Bulboaca I, Lassaut M and Lombard R J 1994 *Proc. 6th Int. Conf. On Clusters in Nuclear Structure and Dynamics (6–9 September 1994, Strasbourg, France)* ed F Haas
[2] Martorell J and Sprung D W L 1992 *Phys. Rev.* B **45** 11 960
[3] Goldstone J and Jaffe R L 1992 *Phys. Rev.* B **45** 14 100
[4] Georgelin Y and Wallet J C 1994 *Phys. Rev.* D **50** 6610
[5] Chadan K and Sabatier P C 1989 *Inverse Problems in Quantum Scattering Theory* 2nd edn (New York: Springer)
[6] Chadan K and Montes Lozano A 1967 *Phys. Rev.* **164** 1762
[7] Abramowitz M and Stegun I A (ed) 1970 *Handbook of Mathematical Functions* 7th edn (New York: Dover)
[8] Erdélyi A 1953 *Higher Transcendental Functions* vol II (New York: McGraw-Hill)
[9] Flügge S 1994 *Practical Quantum Mechanics* 2nd edn (Berlin: Springer)
[10] Chadan K and Musette M 1987 *C. R. Acad. Sci., Paris* **305** 1409
[11] Lombard R J and Moszkowski S A 1994 *Nuovo Cimento* B **109** 1291