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A Zero-Range Model for the Efimov Effect in the Born–Oppenheimer Approximation

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Abstract

In this note we discuss the Efimov effect emerging in a three-particle quantum system with zero-range interactions. In particular, we consider two non-interacting identical bosons plus a different lighter particle such that the interaction between a boson and the light particle is resonant. We also assume the validity of the Born–Oppenheimer approximation. Under these conditions, we show that the three-particle system exhibits infinitely many negative eigenvalues which accumulate at zero and satisfy the universal geometrical law characterising the Efimov effect. The result we find is a generalisation of previous results recently obtained in [17, 28].

Keywords Zero-Range Interactions · Three-Body Hamiltonians · Efimov Effect

Mathematics Subject Classification 81Q10 · 35P20 · 35Q40 · 47B25

1 Introduction

The Efimov effect is an interesting physical phenomenon occurring in three-particle quantum systems in three dimensions [9, 10]. It is characterised by the appearance of an infinite sequence of negative eigenvalues E_n of the three-body Hamiltonian, where $E_n \to 0$ as $n \to \infty$, under the specific condition that the two-particle subsystems have no bound states and at least two of them exhibit a zero-energy resonance or, equivalently, an infinite two-body scattering length. For a review, see *e.g.* [25]. A remarkable feature of this effect is that the distribution of the eigenvalues satisfies the universal geometrical law

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$$\frac{E_n}{E_{n+1}} \;\to\; e^{\frac{2\pi}{s}} \qquad \text{for } n \to \infty\,, \tag{1.1}$$

where the parameter $s > 0$ depends only on the mass ratios and possibly on the statistics of the particles.

For the first experimental evidence of Efimov quantum states we refer to [21].

The mathematical analysis of the Efimov effect was initiated by Yafaev in 1974 [32]. He studied a symmetrised form of the Faddeev equations for the bound states of the three-particle Hamiltonian and proved the existence of an infinite number of negative eigenvalues. In 1993 Sobolev [29] used a slightly different symmetrisation of the equations and proved the following asymptotic behaviour

$$\lim_{z\to 0^-} \frac{N(z)}{|\log|z||} = \frac{s}{2\pi}\,, \tag{1.2}$$

where $N(z)$ denotes the number of eigenvalues smaller than $z < 0$. Note that (1.2) is consistent with the law (1.1). In the same year Tamura [31] obtained the same result under more general conditions on the two-body potentials. Other mathematical proofs of the effect were obtained by Ovchinnikov and Sigal in 1979 [27] and Tamura in 1991 [30] using a variational approach based on the Born–Oppenheimer approximation. Further results on the subject have been obtained in [20], in [4], for the case of two identical fermions and a different particle, and in [19], for a two-dimensional variant of the problem. We stress that a rigorous derivation of the law (1.1) is lacking in the mathematical works mentioned above.

Regarding the Efimov effect, it is also worth mentioning the work of Minlos and Faddeev ([23, 24]) on the problem of defining the Hamiltonian for a system of three bosons with zero-range interactions in three dimensions. They constructed a self-adjoint Hamiltonian by imposing suitable two-body boundary conditions on the coincidence hyperplanes, *i.e.*, where any two particle positions coincide, and a three-body boundary condition at the triple-coincidence point, *i.e.*, where all three particle positions coincide. They also proved that such a Hamiltonian is unbounded from below due to the presence of an infinite sequence of negative eigenvalues diverging to $-\infty$. As a further interesting result, in the case of infinite two-body scattering length (corresponding to the resonant case), they proved the occurrence of the Efimov effect with a rigorous derivation of the law (1.1) (note that the works of Minlos and Faddeev predate those of Efimov). Nevertheless, such a result is somewhat tainted by the fact that the Hamiltonian is unbounded from below and therefore unsatisfactory from the physical point of view.

We mention that the problem of constructing a three-dimensional, lower bounded, zero-range Hamiltonian for a three-body system has been recently approached in the literature. In [16], following a suggestion from [23], an effective three-body force was introduced, acting only when the three particles are close to each other and thereby preventing the fall-to-the-centre phenomenon (sometimes known as the *Thomas effect*). This model was then studied in more detail in [5, 12] and in [22, Section 9] – which introduces different techniques to exhibit the lower bounded, three-body, zero-range Hamiltonian.

Extensions to the many-particle case were developed in [13, 15]: the former concerns non-interacting bosons with a zero-range interacting impurity, while the latter discusses the whole zero-range interacting Bose gas by introducing a four-body repulsion – extending a result contained in [2, Section 2].

In [11], the role of the effective three-body force is played by a three-body hard-core repulsion. It is shown that the Hamiltonian is self-adjoint and bounded from below; moreover, it is also proved that the Efimov effect occurs in the resonant case, *i.e.*, there exists an infinite sequence of negative eigenvalues satisfying (1.1).

In this note, we discuss the approach to the Efimov effect in a three-particle system with zero-range interactions by using the Born–Oppenheimer approximation. Similar approximations have been recently investigated in [17, 28]; see Remark 1 for a more detailed comparison with those results. We also mention [18] for an approach to the Efimov effect in a system with separable potentials and [7] for the analysis of the Born–Oppenheimer approximation in a one dimensional system with point interactions.

More precisely, we consider a system made of two identical scalar bosons with mass M and another different spinless particle with mass m and let $\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3 \in \mathbb{R}^3$ be the coordinates of the bosons and the other particle, respectively. We introduce the system of Jacobi coordinates $\boldsymbol{r}_{\text{cm}}, \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$ defined as

$$\boldsymbol{r}_{\text{cm}} := \frac{M(\boldsymbol{x}_1+\boldsymbol{x}_2)+m\,\boldsymbol{x}_3}{2M+m}\,, \qquad \boldsymbol{y} := \boldsymbol{x}_1-\boldsymbol{x}_2\,, \qquad \boldsymbol{x} := \boldsymbol{x}_3-\frac{\boldsymbol{x}_1+\boldsymbol{x}_2}{2}\,.$$

We study the problem in the centre-of-mass reference frame and we set $\hbar = 1$. The Hilbert space encoding the bosonic symmetry of the system is the following

$$L^2_s(\mathbb{R}^6) := \Big\{\psi \in L^2(\mathbb{R}^6) \;\Big|\; \psi(\boldsymbol{x},\boldsymbol{y}) = \psi(\boldsymbol{x},-\boldsymbol{y})\Big\}\,. \tag{1.3}$$

For simplicity, we also assume that the two identical bosons do not interact. Then the heuristic Hamiltonian describing our three-particle system is expressed by

$$\widetilde{H} = -\frac{1}{\mu}\Delta_{\boldsymbol{y}} - \frac{1}{\nu}\Delta_{\boldsymbol{x}} + \delta(\boldsymbol{x}-\boldsymbol{y}/2) + \delta(\boldsymbol{x}+\boldsymbol{y}/2), \tag{1.4}$$

where

$$\mu = M, \qquad \nu = \frac{4Mm}{2M+m}\,. \tag{1.5}$$

The first step is to give a rigorous meaning to the above formal Hamiltonian on the Hilbert space $L^2_s(\mathbb{R}^6)$. By definition, the Hamiltonian is a self-adjoint extension of the symmetric operator

$$\dot{H}_0 = -\frac{1}{\mu}\Delta_{\boldsymbol{y}} - \frac{1}{\nu}\Delta_{\boldsymbol{x}}\,, \quad D(\dot{H}_0) = \Big\{\psi \in L^2_s(\mathbb{R}^6)\cap H^2(\mathbb{R}^6) \;\Big|\; \psi|_{\pi_\pm} = 0\Big\}\,, \tag{1.6}$$

where

$$\pi_\pm := \Big\{(\boldsymbol{x},\boldsymbol{y}) \in \mathbb{R}^6 \;\Big|\; \boldsymbol{x} = \pm\boldsymbol{y}/2\Big\}\,. \tag{1.7}$$

Using Theorem 2.2 in [13], we consider the bounded from below Hamiltonian H, $D(H)$ in $L^2_s(\mathbb{R}^6)$ satisfying the two conditions:

(C-1) $H\psi = H_0\psi$, where H_0 is the free three-body Hamiltonian, for $\psi \in D(H)$ with $\psi|_{\pi_\pm} = 0$;
(C-2) $\psi \in D(H)$ satisfies the boundary condition on $\pi_\pm$

$$\psi(\boldsymbol{x}, \boldsymbol{y}) = \frac{\xi(\pm\boldsymbol{y})}{|\boldsymbol{x} \mp \boldsymbol{y}/2|} + \left(\alpha + \frac{\theta(|\boldsymbol{y}|)}{|\boldsymbol{y}|}\right)\xi(\pm\boldsymbol{y}) + o(1) \qquad \text{for } \boldsymbol{x} \to \pm\boldsymbol{y}/2, \tag{1.8}$$

where

$$\xi(\boldsymbol{y}) := \lim_{\boldsymbol{x}\to\boldsymbol{y}/2} |\boldsymbol{x} - \boldsymbol{y}/2|\,\psi(\boldsymbol{x}, \boldsymbol{y}), \tag{1.9}$$

$\alpha \in \mathbb{R}$, and $\theta : \mathbb{R}^+ \longrightarrow \mathbb{R}$ is smooth and satisfies the conditions

$$\theta(0) = 1\,, \qquad \theta(r) = 0 \quad \text{for} \quad r \geq r_0 > 0.$$

The parameter α is the inverse of the two-body scattering length. Moreover, the role of the function $\theta/|\cdot|$ is to regularise the interaction when the positions of the three particles coincide, thereby preventing the fall-to-centre phenomenon (for additional technical details, we refer to [13]). Notice that r_0 can be chosen to be arbitrarily small.

Our aim is to study the eigenvalue problem

$$H\Psi = E\Psi\,, \qquad E < 0 \tag{1.10}$$

and the occurrence of the Efimov effect for the Hamiltonian H, $D(H)$ under the two assumptions:

- $\alpha = 0$, *i.e.*, for an infinite two-body scattering length,
- $M \gg m$ (equivalently, $\mu \gg \nu$).

More precisely, in this note we assume the validity of the Born–Oppenheimer approximation, which means that

$$E \simeq E_{\mathrm{BO}}\,, \qquad \Psi(\boldsymbol{x}, \boldsymbol{y}) \simeq \zeta(\boldsymbol{y})\phi(\boldsymbol{x}; \boldsymbol{y}) \tag{1.11}$$

where, for any fixed $\boldsymbol{y}$, $\phi(\cdot\,; \boldsymbol{y})$ is an eigenvector with eigenvalue $\mathcal{E}(|\boldsymbol{y}|)$ of the formal one-body Hamiltonian with two point interactions placed at $\pm\boldsymbol{y}/2$

$$\widetilde{h}(\boldsymbol{y}) = -\frac{1}{\nu}\Delta + \delta(\cdot - \boldsymbol{y}/2) + \delta(\cdot + \boldsymbol{y}/2), \tag{1.12}$$

and ζ is an eigenvector with eigenvalue E_{BO} of the one-body Hamiltonian

$$h_{\mathcal{E}} = -\frac{1}{\mu}\Delta + \mathcal{E}(|\cdot|). \tag{1.13}$$

Hence, the problem is reduced to first solving the eigenvalue problem for the fast dynamics associated with (1.12), and then treating the resulting eigenvalue $\mathcal{E}(|\boldsymbol{y}|)$ as an effective potential for the slow dynamics described by (1.13).

It is important to stress that the one-body Hamiltonian $\widetilde{h}(\boldsymbol{y})$ is obtained by freezing the slow dynamics in the three-body Hamiltonian H (for $\alpha = 0$) and then considering the coordinate $\boldsymbol{y}$ as a fixed parameter. Hence, the rigorous counterpart $h(\boldsymbol{y})$, $D(h(\boldsymbol{y}))$ of (1.12) (see (2.1), (2.2)) is a self-adjoint and bounded from below operator in $L^2(\mathbb{R}^3)$ satisfying the two conditions:

(c-1) $h(\boldsymbol{y})u = h_0 u$, where $h_0 = -\frac{1}{\nu}\Delta$ is the free one-body Hamiltonian, for $u \in D(h(\boldsymbol{y}))$ with $u(\pm\boldsymbol{y}/2) = 0$;
(c-2) $u \in D(h(\boldsymbol{y}))$ satisfies the boundary condition at $\boldsymbol{x} = \pm\boldsymbol{y}/2$

$$u(\boldsymbol{x}) = \frac{q}{|\boldsymbol{x} \mp \boldsymbol{y}/2|} + \frac{\theta(|\boldsymbol{y}|)}{|\boldsymbol{y}|} q + o(1) \qquad \text{for } \boldsymbol{x} \to \pm\boldsymbol{y}/2, \tag{1.14}$$

where

$$q := \lim_{\boldsymbol{x} \to \boldsymbol{y}/2} |\boldsymbol{x} - \boldsymbol{y}/2|\, u(\boldsymbol{x}). \tag{1.15}$$

Such an operator is known as a Hamiltonian with non-local point interactions at the points $\pm\boldsymbol{y}/2$, and its main properties are recalled in the next section.

The eigenvalues E_{BO} of the one-body Hamiltonian $h_{\mathcal{E}}$ are usually assumed to be a good approximation of the true eigenvalues E of the three-body Hamiltonian H, $D(H)$ for $M \gg m$. A rigorous proof of this fact is not discussed in this note, and it will be addressed in a future work.

The next theorem summarises our main result.

Theorem 1.1 *The following two statements hold:*

(i) for any fixed $\boldsymbol{y} \in \mathbb{R}^3$*, the Hamiltonian* $h(\boldsymbol{y})$ *defined in* (2.1)*,* (2.2) *admits the negative eigenvalue*

$$\mathcal{E}(|\boldsymbol{y}|) = -\frac{\left(W\left(e^{\theta(|\boldsymbol{y}|)}\right) - \theta(|\boldsymbol{y}|)\right)^2}{\nu|\boldsymbol{y}|^2}, \tag{1.16}$$

where $W : \left[-\frac{1}{e}, \infty\right) \longrightarrow [-1, \infty)$ *denotes the principal branch of the Lambert function;*

(ii) the Hamiltonian $h_{\mathcal{E}}$ *introduced in* (1.13) *admits an infinite sequence of negative eigenvalues* $\{E_{\mathrm{BO};\,n}\}_{n\in\mathbb{N}}$*, such that* $\lim_{n\to\infty} E_{\mathrm{BO};\,n} = 0$ *and*

$$\lim_{n\to\infty} \frac{E_{\mathrm{BO};\,n}}{E_{\mathrm{BO};\,n+1}} = e^{\frac{2\pi}{\beta}}, \tag{1.17}$$

where $\beta = \sqrt{\frac{\mu}{\nu} W(1)^2 - \frac{1}{4}}$ *and* $W(1) \simeq 0.567143$.

Remark 1 The result expressed in Theorem 1.1 is essentially the same as that found in [17, 28]. The only difference is that in these latter works our function θ is replaced by the function

$$g(r) = e^{-r/\sqrt{2}}\Big(\sin\frac{r}{\sqrt{2}} + \cos\frac{r}{\sqrt{2}}\Big).$$

Such a function emerges as a specific choice in the construction of the one-body Hamiltonian $h(\boldsymbol{y})$ with (non-local) point interactions placed at $\boldsymbol{x} = \pm\boldsymbol{y}/2$ in the context of the theory of self-adjoint extensions. On the contrary, we derive our model from a full three-body problem and the Hamiltonian $h(\boldsymbol{y})$ is therefore regarded and obtained as the limit for $M \to \infty$ of the three-body Hamiltonian H (see [14, Section 4]). In this sense we believe that our approach here is more natural from the physical point of view and, moreover, the result is slightly more general, since it holds for any choice of the function θ satisfying the properties stated above. As expected, the explicit choice of θ – encoding the microscopic interaction around the singularity at the triple coincidence point – does not appear in the asymptotic geometrical law (1.17) resulting from the long-range behaviour of the effective three-body interaction.

The proof of Theorem 1.1 will be given in the following two sections.

In Sect. 2 we recall definition and main properties of the Hamiltonian $h(\boldsymbol{y})$ and then solve the corresponding eigenvalue problem. In particular, we compute the eigenvalue $\mathcal{E}(|\boldsymbol{y}|)$ and the corresponding eigenfunction.

In Sect. 3 we study the eigenvalue problem for $h_{\mathcal{E}}$, showing that there is an infinite sequence of negative eigenvalues accumulating at zero and satisfying the asymptotic law (1.17). The corresponding eigenfunctions are also explicitly characterised. Our proof relies on elementary and explicit computations exploiting the $\frac{1}{r^2}$ decay of the effective potential $\mathcal{E}$. For a possible alternative approach, based on a WKB argument, we refer to the physics paper [6].

2 Fast Dynamics

We start this section giving the rigorous definition of the operator formally written in (1.12). Let

$$G^{\lambda}(\boldsymbol{x}) = \frac{e^{-\sqrt{\lambda\nu}|\boldsymbol{x}|}}{|\boldsymbol{x}|}$$

for $\lambda > 0$, be the solution to $(-\frac{1}{\nu}\Delta + \lambda)G^{\lambda} = \frac{4\pi}{\nu}\delta_{\boldsymbol{0}}$ normalised so that it has the desired singular behaviour

$$G^{\lambda}(\boldsymbol{x}) = \frac{1}{|\boldsymbol{x}|} - \sqrt{\lambda\nu} + o(1)$$

as $\boldsymbol{x} \to 0$. The rigorous definition of the operator $h(\boldsymbol{y})$ is given by Theorem 1.1.3 in [1] (we restrict our attention to functions symmetric in the exchange of the scatterer positions due to the symmetry of the three-body problem, see (1.3)). We also refer to [17, Lemma 3.2] where the operator with (non-local) point interactions placed at $\pm\boldsymbol{y}/2$ is obtained from the general theory in [8]. We get

$$D(h(\boldsymbol{y})) = \Big\{u \in L^2(\mathbb{R}^3) : u = \omega^\lambda + q\, G^\lambda(\cdot + \boldsymbol{y}/2) + q\, G^\lambda(\cdot - \boldsymbol{y}/2),\ q \in \mathbb{C},\ \omega^\lambda \in H^2(\mathbb{R}^3),$$
$$\omega^\lambda\big(\pm \boldsymbol{y}/2\big) = q\Big(\frac{\theta(|\boldsymbol{y}|)}{|\boldsymbol{y}|} + \sqrt{\lambda\nu} - G^\lambda(\boldsymbol{y})\Big)\Big\}. \tag{2.1}$$

The action of $h(\boldsymbol{y})$ on $u \in D(h(\boldsymbol{y}))$ is given by

$$(h(\boldsymbol{y}) + \lambda)u = (h_0 + \lambda)\omega^\lambda \tag{2.2}$$

where $h_0 = -\frac{1}{\nu}\Delta$. Notice that the last equality in (2.1) rephrases the boundary condition (1.14), (1.15) and, moreover, if $u \in D(h(\boldsymbol{y}))$ and $u(\pm\boldsymbol{y}/2) = 0$ then (2.2) implies $h(\boldsymbol{y})u = h_0 u$. Hence the two conditions (c-1), (c-2) stated in the Introduction are satisfied.

The operator in $L^2(\mathbb{R}^3)$ defined by (2.1), (2.2) is self-adjoint and bounded from below and it is known in the literature as a Schrödinger operator with non-local point interactions at $\pm\boldsymbol{y}/2$. The non-local character is due to the presence of the function θ which makes the boundary condition, and therefore the strength of the interaction, dependent on the distance of the two point interactions. Notice that the form chosen for the function θ is such that the boundary condition remains well defined in the limit $|\boldsymbol{y}| \to 0$ (whereas if $\theta = 0$ it loses its meaning in the limit).

The Hamiltonian $h(\boldsymbol{y})$ defines a solvable model, in the sense that the spectrum and the (proper and generalised) eigenfunctions can be explicitly characterised. In particular, it is easy to check that $h(\boldsymbol{y})$ does not have any positive eigenvalues. Let's now show the existence of a negative eigenvalue. Assume $-\lambda < 0$ is an eigenvalue and let $\phi = \omega^\lambda + q\Big(G^\lambda(\cdot + \boldsymbol{y}/2) + G^\lambda(\cdot - \boldsymbol{y}/2)\Big) \in D(h(\boldsymbol{y}))$ be the corresponding eigenvector. Equation (2.2) immediately yields $(h_0 + \lambda)\omega^\lambda = 0$, and therefore $\omega^\lambda = 0$. Thus, by the boundary condition in (2.1) we conclude that λ is a solution of the equation

$$\frac{\theta(|\boldsymbol{y}|)}{|\boldsymbol{y}|} + \sqrt{\nu\lambda} - G^\lambda(\boldsymbol{y}) = 0.$$

Introducing the new variable $s = \sqrt{\nu\lambda}|\boldsymbol{y}| + \theta(|\boldsymbol{y}|)$ and recalling the expression of G^λ we rewrite the equation as

$$s e^s = e^{\theta(|\boldsymbol{y}|)}.$$

Since $e^{\theta(|\boldsymbol{y}|)} > 0$, the only solution to the above equation is given by $s = W(e^{\theta(|\boldsymbol{y}|)})$ with W the principal branch of the Lambert function defined as $W = f^{-1}$ with $f(s) = s e^s, s \geq -1$. Note that W is smooth, non-negative, and increasing, with $W(e) = 1$. We conclude that the only eigenvalue of the operator $h(\boldsymbol{y})$ is

$$\mathcal{E}(|\boldsymbol{y}|) = -\lambda = -\frac{\Big(W(e^{\theta(|\boldsymbol{y}|)}) - \theta(|\boldsymbol{y}|)\Big)^2}{\nu|\boldsymbol{y}|^2}.$$

In particular, recalling the assumption on θ, we have that $\mathcal{E}(|\boldsymbol{y}|) = -\frac{W(1)^2}{\nu|\boldsymbol{y}|^2}$ for $|\boldsymbol{y}| \geq r_0$. Moreover, for $|\boldsymbol{y}| < r_0$ we have that $\mathcal{E}(|\boldsymbol{y}|)$, whose exact expression depends on θ, is always continuous and bounded. The corresponding eigenvector is

$$\phi(\cdot\,;\boldsymbol{y}) = q\Big(G^{-\mathcal{E}(|\boldsymbol{y}|)}(\cdot + \boldsymbol{y}/2) + G^{-\mathcal{E}(|\boldsymbol{y}|)}(\cdot - \boldsymbol{y}/2)\Big)$$

with q normalising constant.

It is important to stress once again the regularising role of the function θ. Indeed, in the case $\theta = 0$ the eigenvalue would reduce to $\mathcal{E}(|\boldsymbol{y}|) = -\frac{W(1)^2}{\nu|\boldsymbol{y}|^2}$ for any $\boldsymbol{y} \in \mathbb{R}^3$ and therefore the potential $\mathcal{E}(|\boldsymbol{y}|)$ for the slow dynamics would be too singular for $\boldsymbol{y} \to 0$.

3 Slow Dynamics

Here we study the eigenvalue problem for the one-body Hamiltonian

$$h_{\mathcal{E}} = -\frac{1}{\mu}\Delta + \mathcal{E}(|\cdot|)\,, \qquad D(h_{\mathcal{E}}) = H^2(\mathbb{R}^3)$$

where $\mathcal{E}(|\cdot|)$ is the continuous and bounded function given by (1.16). When the angular momentum between the two heavy particles is large, the associated centrifugal contribution – that decays as $\frac{1}{r^2}$ – competes with the potential possibly forbidding the emergence of the infinite sequence of eigenvalues accumulating at zero. It is therefore natural restricting the analysis to the s-wave sector and the problem to be solved is

$$\begin{cases} -\zeta''(r) - \dfrac{2}{r}\zeta'(r) + \mu\,\mathcal{E}(r)\zeta(r) = \mu\, E_{\mathrm{BO}}\,\zeta(r), & \min\mathcal{E} \le E_{\mathrm{BO}} < 0,\ r \in \mathbb{R}_+, \\ r\,\zeta(r) \in H^2(\mathbb{R}_+). \end{cases} \tag{3.1}$$

Recall that $H^2(\mathbb{R}^3) \subset C^0(\mathbb{R}^3)$: specifically, ζ is finite at every point.
Consider the substitution $u : r \longmapsto r\,\zeta(r) \in H^2(\mathbb{R}_+) \cap H_0^1(\mathbb{R}_+)$ and the notation $\lambda := \sqrt{-\mu\,E_{\mathrm{BO}}}$, and $\beta := \sqrt{\frac{\mu\,W(1)^2}{\nu} - \frac{1}{4}}$. Then, (3.1) reads

$$\begin{cases} u'' - (\mu\,\mathcal{E} + \lambda^2)u = 0, \\ u \in H^2(\mathbb{R}_+) \cap H_0^1(\mathbb{R}_+). \end{cases} \tag{3.2}$$

In other words, denoting

$$v(r) = \mu\,\mathcal{E}(r)\,, \qquad 0 \le r \le r_0$$

we arrive at

$$u''(r) - \big(v(r) + \lambda^2\big)u(r) = 0, \qquad 0 < r \le r_0, \tag{3.3}$$

$$u''(r) + \frac{\beta^2 + {}^1\!/_4}{r^2}\,u(r) - \lambda^2 u(r) = 0, \qquad r > r_0, \tag{3.4}$$

with the boundary condition $u(0) = 0$.
Since v is continuous, one finds that $\lambda \longmapsto w_\lambda \in C^0\big([0,\infty), C^2([0,r_0])\big)$ is a solution to equation (3.3) with $w_\lambda(0) = 0$ and[1] $w'_\lambda(0) = c \neq 0$. Such a solution exists and is unique by the Picard–Lindelöf theorem. In particular, it follows that

$$w_\lambda(r) = w_0(r) + R_\lambda(r), \qquad \text{with} \lim_{\lambda\to 0^+} \|R_\lambda\|_{C^2([0,r_0])} = 0.$$

Indeed one can write (3.3) in its integral form

$$u(r) = c\,r + \int_0^r ds\ (r-s)\big(v(s)+\lambda^2\big)u(s).$$

Therefore, by Grönwall's lemma,

$$|w_\lambda(r)| \le c\,r\,e^{\frac{1}{2}r^2\left(\|v\|_\infty + \lambda^2\right)},$$
$$|w_\lambda(r) - w_{\lambda'}(r)| \le \int_0^r ds\ (r-s)\big(|v(s)|+\lambda^2\big)|w_\lambda(s)-w_{\lambda'}(s)| + \frac{c\,|\lambda^2-\lambda'^2|\,r}{\|v\|_\infty+\lambda'^2}\,e^{\frac{1}{2}r^2\left(\|v\|_\infty+\lambda'^2\right)},$$

which implies

$$\sup_{r\in[0,r_0]} |w_\lambda(r) - w_{\lambda'}(r)| \le \frac{c\,|\lambda^2-\lambda'^2|\,r_0}{\|v\|_\infty+\lambda'^2}\,e^{r_0^2\left(\|v\|_\infty+\frac{\lambda^2+\lambda'^2}{2}\right)},$$

and the (Lipschitz) continuity in $\lambda \in [0,\infty)$ follows. A similar argument holds for w'_λ. In conclusion, the linearity of the ODE and the smoothness in λ of the coefficients guarantee that $w''_\lambda = (v+\lambda^2)\,w_\lambda$ is continuous in λ as well (actually, one therefore has $\lambda \longmapsto w_\lambda \in C^\infty([0,\infty), C^2([0,r_0]))$. However, we point out that our problem involves values of λ in the interval $\big(0,\ \|v\|_\infty^{1/2}\,\big]$.

As an explicit example, consider $v \equiv -\lambda_0^2 := -\frac{\beta^2+1/4}{r_0^2}$; in this case, one has $0 < \lambda \le \lambda_0$ and

$$w_\lambda(r) = \begin{cases} c\,r, & \lambda = \lambda_0, \\ \dfrac{c\,\sin(\lambda_0 r)}{\lambda_0} + R_\lambda(r), & \lambda < \lambda_0, \end{cases} \qquad \text{with } R_\lambda(r) = \frac{c\,\sin\!\left(\sqrt{\lambda_0^2-\lambda^2}\,r\right)}{\sqrt{\lambda_0^2-\lambda^2}} - \frac{c\,\sin(\lambda_0 r)}{\lambda_0}.$$

Next, the second-order ODE (3.4) can be solved explicitly; moreover, only one of the independent solutions decays at infinity, *i.e.*

$$r \longmapsto \sqrt{r}\,K_{i\beta}(\lambda r).$$

Here, $K_{i\beta}$ is the modified Bessel function of the second kind, sometimes also known as the Macdonald function, which satisfies the following asymptotic behaviours (see [26,

[1] Observe that the value of w'_λ at zero corresponds to that of the function ζ at the origin.

eq. 10.40.2 p. 255, eq. 10.45.7 p. 261])

$$K_{i\beta}(z) = \sqrt{\tfrac{\pi}{2z}}\, e^{-z}\Big[1 - \tfrac{4\beta^2+1}{8z} + O(z^{-2})\Big], \qquad \text{for } z \to +\infty, \tag{3.5a}$$

$$K_{i\beta}(z) = -\sqrt{\tfrac{\pi}{\beta \sinh(\pi\beta)}}\, \sin\!\big(\beta \log \tfrac{z}{2} - \vartheta_\beta\big) + O(z^2), \qquad \text{for } z \to 0^+, \tag{3.5b}$$

with $\vartheta_\beta := \arg \Gamma(1 + i\beta) \in (-\pi, \pi]$.
Hence, the problem (3.2) has the following solution:

$$u_\lambda(r) = \begin{cases} A\, w_\lambda(r), & 0 \le r \le r_0, \\ B \sqrt{r}\, K_{i\beta}(\lambda r), & r > r_0, \end{cases} \tag{3.6}$$

with A, B proper constants such that

$$\lim_{r \to r_0^-} u_\lambda(r) = \lim_{r \to r_0^+} u_\lambda(r), \qquad \lim_{r \to r_0^-} u'_\lambda(r) = \lim_{r \to r_0^+} u'_\lambda(r).$$

The previous matching condition is due to the embedding $H^2(\mathbb{R}) \hookrightarrow C^1(\mathbb{R})$. Therefore, one must require

$$\begin{cases} w_\lambda(r_0)\, A - \sqrt{r_0}\, K_{i\beta}(\lambda r_0)\, B = 0, \\ w'_\lambda(r_0)\, A - \left[\dfrac{1}{2\sqrt{r_0}} K_{i\beta}(\lambda\, r_0) + \lambda \sqrt{r_0}\, K'_{i\beta}(\lambda r_0)\right] B = 0. \end{cases} \tag{3.7}$$

In order to exclude the identically zero solution $u_\lambda \equiv 0$, one cannot admit $A = B = 0$. Consequently, the matrix associated with the previous linear system of equations must be singular:

$$-w_\lambda(r_0) \left[\frac{1}{2\sqrt{r_0}} K_{i\beta}(\lambda\, r_0) + \lambda \sqrt{r_0}\, K'_{i\beta}(\lambda r_0)\right] + \sqrt{r_0}\, K_{i\beta}(\lambda r_0)\, w'_\lambda(r_0) = 0,$$

namely,

$$\left[\frac{w_\lambda(r_0)}{2} - r_0\, w'_\lambda(r_0)\right] K_{i\beta}(\lambda\, r_0) + \lambda r_0\, w_\lambda(r_0)\, K'_{i\beta}(\lambda r_0) = 0. \tag{3.8}$$

Our goal is to prove that (3.8) can be solved for infinitely many energy levels accumulating at zero according to Efimov’s asymptotic geometrical law.
Combining [26, eqs. 10.27.3, 10.29.1, and 10.30.2], one can compute the asymptotic expansion for the derivative of the Macdonald function as $z \to 0^+$

$$\begin{aligned} K'_{i\beta}(z) &= -\frac{1}{2z}\left[\Gamma(1-i\beta)(\tfrac{1}{2}z)^{i\beta} + \Gamma(1+i\beta)(\tfrac{1}{2}z)^{-i\beta}\right] + O(z) \\ &= -\frac{|\Gamma(1+i\beta)|}{2z}\left[e^{-i\vartheta_\beta}\, e^{i\beta \ln(\frac{1}{2}z)} + e^{i\vartheta_\beta}\, e^{-i\beta \ln(\frac{1}{2}z)}\right] + O(z), \end{aligned}$$

where we have used $\Gamma(\bar{z}) = \overline{\Gamma(z)}$. Hence, by exploiting [3, eq. 5.4.3 p. 137] for the absolute value of the Gamma function, one gets

$$z\,K'_{i\beta}(z) = -\sqrt{\tfrac{\pi\beta}{\sinh(\pi\beta)}}\,\cos\!\big(\beta\ln\tfrac{z}{2} - \vartheta_\beta\big) + O(z^2), \qquad \text{for } z \to 0^+. \tag{3.9}$$

Introducing the parameters

$$a := \frac{w_0(r_0)}{2} - r_0\,w_0'(r_0), \qquad\qquad b := \beta\,w_0(r_0), \tag{3.10}$$

condition (3.8) can be equivalently rewritten as

$$-\,a\sin\!\big(\vartheta_\beta - \beta\ln\tfrac{\lambda r_0}{2}\big) + b\cos\!\big(\vartheta_\beta - \beta\ln\tfrac{\lambda r_0}{2}\big) = F_{r_0}(\lambda), \tag{3.11}$$

for some continuous function $F_{r_0} : \mathbb{R}_+ \longrightarrow \mathbb{R}$ satisfying

$$\lim_{\lambda\to 0^+} F_{r_0}(\lambda) = 0, \qquad \text{for all } r_0 \in \mathbb{R}_+.$$

We stress that a and b cannot both be equal to zero. Otherwise, it follows that $w_0(r_0) = w_0'(r_0) = 0$, and the initial value problem (3.3) for $\lambda = 0$ with such conditions has the identically zero function as a solution. By uniqueness, $w_0(r) = 0$ for all $r \in [0, r_0]$, contradicting $w'_\lambda(0) \neq 0$.

Let us solve (3.11) in the case where F_{r_0} is replaced by zero:

$$\begin{aligned} &-a\sin\!\big(\vartheta_\beta - \beta\ln\tfrac{\lambda r_0}{2}\big) + b\cos\!\big(\vartheta_\beta - \beta\ln\tfrac{\lambda r_0}{2}\big) = 0 \\ \Longleftrightarrow\;& \tan\big(\vartheta_\beta - \beta\ln\tfrac{\lambda r_0}{2}\big) = \frac{b}{a}, \qquad \text{provided } a \neq 0, \end{aligned} \tag{3.12}$$

thus,

$$\begin{aligned} &\vartheta_\beta - \beta\ln\tfrac{\lambda r_0}{2} = \arctan\tfrac{b}{a} + n\pi, \qquad n \in \mathbb{Z} \\ \Longrightarrow\;& \lambda_n^0 = \tfrac{2}{r_0}\,e^{\frac{\vartheta_\beta-\alpha}{\beta}}\,e^{-n\frac{\pi}{\beta}}, \qquad \alpha := \arctan\tfrac{b}{a}. \end{aligned} \tag{3.13}$$

Note that $\alpha = 0$ in the case $b = 0$, while (3.13) remains valid for $a = 0$ upon choosing $\alpha = \frac{\pi}{2}$. In the following, we show that equation (3.11) admits infinitely many solutions λ_n with the same asymptotic behaviour as λ_n^0 as $n \to +\infty$.
To this end, let us consider the equation

$$\sin\eta = \frac{(-1)^n}{\sqrt{a^2+b^2}}\,F_{r_0}\big(\lambda_n^0\,e^{\frac{\eta}{\beta}}\big), \qquad \eta \in \big(-\tfrac{\pi}{2}, \tfrac{\pi}{2}\big). \tag{3.14}$$

Since $\lambda_n^0 e^{\frac{\eta}{\beta}} \in \left(\lambda_n^0 e^{-\frac{\pi}{2\beta}}, \lambda_n^0 e^{\frac{\pi}{2\beta}}\right)$ and $\lim_{n\to+\infty} F_{r_0}\left(\lambda_n^0 e^{\frac{\eta}{\beta}}\right) = 0$, there exists $n_0 = n_0(v, r_0, \beta) \in \mathbb{Z}$ such that

$$\frac{|F_{r_0}\left(\lambda_n^0 e^{\frac{\eta}{\beta}}\right)|}{\sqrt{a^2+b^2}} < 1, \qquad \forall n \geq n_0.$$

Therefore, for all $n \geq n_0$, (3.14) has a unique solution $\eta_n \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$ satisfying $\lim_{n\to+\infty} \eta_n = 0$.

We now have all the elements required to prove the following proposition.

Proposition 3.1 *Let $\lambda_n^0 \in \mathbb{R}_+$ be a solution to (3.12). Then, there exists $n_0 = n_0(v, r_0, \beta) \in \mathbb{Z}$ such that if $n \geq n_0$, there exists a unique solution $\eta_n \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$ to (3.14), with a, b given by (3.10). Moreover, equation (3.8) admits infinitely many solutions of the form*

$$\lambda_n = \lambda_n^0 e^{\eta_n/\beta}, \qquad n \geq n_0. \tag{3.15}$$

Proof We have already discussed the existence and uniqueness of η_n; therefore, we focus on the proof of (3.15). Equation (3.8) is equivalent to (3.11), which can, in turn, be rewritten by replacing λ with $\lambda_n^0 e^{\frac{\eta_n}{\beta}}$

$$-a \sin(\alpha + n\pi - \eta_n) + b\cos(\alpha + n\pi - \eta_n) = F_{r_0}\left(\lambda_n^0 e^{\frac{\eta_n}{\beta}}\right).$$

Hence,

$$-a\left(\sin\alpha \cos\eta_n - \cos\alpha \sin\eta_n\right) + b\left(\cos\alpha \cos\eta_n + \sin\alpha \sin\eta_n\right) = (-1)^n F_{r_0}\left(\lambda_n^0 e^{\frac{\eta_n}{\beta}}\right).$$

Since $-a\sin\alpha + b\cos\alpha = 0$ (see (3.12)), one has

$$\left(a\cos\alpha + b\sin\alpha\right)\sin\eta_n = (-1)^n F_{r_0}\left(\lambda_n^0 e^{\frac{\eta_n}{\beta}}\right). \tag{3.16}$$

Lastly, exploiting the identities

$$\cos\alpha = \frac{a}{\sqrt{a^2+b^2}}, \quad \sin\alpha = \frac{b}{\sqrt{a^2+b^2}},$$

it is straightforward that (3.16) is equivalent to (3.14) with $\eta = \eta_n$; moreover, (3.14) is automatically solved for $n \geq n_0$. This concludes the proof.

□

The preceding analysis yields the following proposition.

Proposition 3.2 *Using the notation of Proposition 3.1, the eigenvalue problem (3.1) has infinitely many negative solutions $\{E_{\mathrm{BO};\,n}\}_{n=n_0}^{\infty}$, with $\lim_{n\to\infty} E_{\mathrm{BO};\,n} = 0$. Moreover, for all $n \geq n_0$*

$$E_{\mathrm{BO};\,n} = -\frac{4}{\mu r_0^2}\, e^{\frac{2}{\beta}\left(\vartheta_\beta - \arctan\frac{b}{a} + \eta_n\right)}\, e^{-\frac{2\pi}{\beta}n}$$

and the corresponding eigenfunction is

$$u_n(r) = \begin{cases} A_n\, w_{\lambda_n}(r), & 0 \le r \le r_0, \\ B_n \sqrt{r}\, K_{i\beta}(\lambda_n r), & r > r_0 \end{cases}$$

where

$$A_n = \begin{cases} \dfrac{\sqrt{r_0}}{w_{\lambda_n}(r_0)}\, K_{i\beta}(\lambda_n r_0)\, B_n, & \text{if } w_{\lambda_n}(r_0) \neq 0, \\ \dfrac{K_{i\beta}(\lambda_n r_0) + 2\lambda_n r_0\, K'_{i\beta}(\lambda_n r_0)}{2\sqrt{r_0}\, w'_{\lambda_n}(r_0)}\, B_n, & \text{if } w_{\lambda_n}(r_0) = 0, \end{cases}$$

and B_n is the normalisation constant.

Proof The result is derived from Proposition 3.1 and by observing that combining the assumption $u'_\lambda(0) \neq 0$ (implying $w_\lambda(r_0) \neq 0 \vee w'_\lambda(r_0) \neq 0$) with equation (3.8), the linear system (3.7) has a corresponding coefficient matrix of rank 1.

□

As a consequence of the previous proposition, one obtains the proof of the asymptotic geometrical behaviour of the energy levels in the Born–Oppenheimer approximation

$$\lim_{n\to\infty} \frac{E_{\mathrm{BO};\,n}}{E_{\mathrm{BO};\,n+1}} = \lim_{n\to\infty} e^{\frac{2}{\beta}(\eta_n - \eta_{n+1})}\, e^{\frac{2\pi}{\beta}} = e^{2\pi/\beta}.$$

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Declarations

Conflicts of Interest The authors declare that they have no competing interests regarding the publication of this paper.

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