Self-adjoint extensions and spectral analysis in the generalized Kratzer problem

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Abstract

We present a mathematically rigorous quantum-mechanical treatment of a one-dimensional nonrelativistic motion of a particle in the potential field

$$V(x) = g_1 x^{-1} + g_2 x^{-2}, \ x \in \mathbb{R}_+ = [0, \infty) \ .$$

For $g_2 > 0$ and $g_1 < 0$, the potential is known as the *Kratzer potential* $V_K(x)$ and is usually used to describe molecular energy and structure, interactions between different molecules, and interactions between non-bonded atoms.

We construct all self-adjoint Schrödinger operators with the potential V(x) and represent rigorous solutions of the corresponding spectral problems. Solving the first part of the problem, we use a method of specifying s.a. extensions by (asymptotic) s.a. boundary conditions. Solving spectral problems, we follow the Krein's method of guiding functionals. This work is a continuation of our previous works devoted to Coulomb, Calogero, and Aharonov-Bohm potentials.

1 Introduction

In this article, we present a mathematically rigorous quantum-mechanical (QM) treatment of a one-dimensional nonrelativistic motion on a semiaxis of a spinless particle of mass m in the potential field

$$V(x) = g_1 x^{-1} + g_2 x^{-2}, \ x \in \mathbb{R}_+ = [0, \infty) \ .$$
 (1)

On the physical level of rigor, the Schrödinger equation with potential (1) was studied for a long time in connection with different physical problems, see for example [3, 7] and books [10, 8]. In particular, this potential enters the stationary radial Schrödinger equation

$$\left[\frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \left(E_{nl} - U(r) - \frac{l(l+1)\hbar^2}{2mr^2} \right) \right] \psi_{nl}(r) = 0 , \qquad (2)$$

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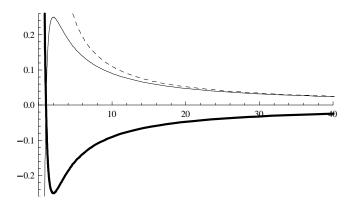


Figure 1: Potential $V(x) = g_1 x^{-1} + g_2 x^{-2}$, with $g_1 = g_2 = 1$ (dashed), $g_1 = -g_2 = 1$ (solid) and $g_1 = -g_2 = -1$ (thick).

where n and l are radial and angular quantum numbers, after separating spherical variables in three-dimensional spherically symmetric QM problems, see e.g. [8]. The potential (1) is singular at the origin, it is repulsive at this point for $g_2 > 0$, and has a minimum at a point $x_0 > 0$ for $g_2 > 0$ and $g_1 < 0$. The potential with g_1, g_2 in the latter range is known as the Kratzer potential [1]. The Kratzer potential is conventionally used to describe molecular energy and structure, interactions between different molecules [5], and interactions between nonbonded atoms [2]. For $g_2 < 0$ and $g_1 > 0$, we have the inverse Kratzer potential which is conventionally used to describe tunnel effects, scattering of charged particles [11] and decays, in particular, molecule ionization and fluorescence [4]. In addition, valence electrons in a hydrogen-like atom are described in terms of such a potential [9]. When modeling some physical systems, a constant is usually added to the angular momentum term, $l(l+1) \rightarrow \beta + l(l+1)$, in order to take some effective potential energy into account. For example, in the model of a molecule interaction, β can represent the dissociation energy of a diatomic molecule [5] or, in the scattering problem, this parameter represents attractive ($\beta < 0$) or repulsive ($\beta > 0$) interactions between charged particles [11].

In Figure 1 we show the shape of the potential under consideration for different values of the parameters.

Even though a number of works was devoted to the QM problem with the potential (1), a rigorous mathematical analysis of this problem is lacking in the literature. The aim of such an analysis (which is, in fact, the aim of the present article) is to construct all self-adjoint (s.a. in what follows) Schrödinger operators (Hamiltonians) with the potential (1) and present rigorous solutions of the corresponding spectral problems.

When solving the first part of the problem, we use a method for specifying s.a. differential operators by (asymptotic) s.a. boundary conditions (the so-

called alternative method, see [12]). When solving spectral problems, we follow the Krein's method of guiding functionals, see [14] and books [15]. This work is a continuation of our previous works [24, 25] devoted to Coulomb, Calogero, and Aharonov-Bohm potentials; using the given references, the reader can become acquainted with necessary basic notions and constructions, like guiding functional and Green function.

As in the above-mentioned works, we start with a s.a. differential operation \check{H} on \mathbb{R}_+ ,

$$\check{H} = -d_x^2 + g_1 x^{-1} + g_2 x^{-2},\tag{3}$$

and examining solutions of the corresponding homogeneous differential equation $(\check{H} - W)\psi = 0$, or

$$\psi'' - (g_1 x^{-1} + g_2 x^{-2} - W)\psi = 0, \ W = |W|e^{i\varphi}, \ 0 \le \varphi < 2\pi \ , \tag{4}$$

which is the Schrödinger equation (with omitted factor $2m/\hbar^2$) with a complex energy W, for Im W = 0, we write W = E in what follows.

The basic operator \hat{H}^+ in $L^2(\mathbb{R}_+)$ associated with \check{H} is defined on the natural domain $D_{\check{H}}^*(\mathbb{R}_+) \subset L^2(\mathbb{R}_+)$,

$$D_{\check{H}}^{*}\left(\mathbb{R}_{+}\right) = \left\{\psi_{*}(x) : \psi_{*}, \psi_{*}' \text{ are a.c. in } \mathbb{R}_{+}; \psi_{*}, \check{H}\psi_{*} \in L^{2}\left(\mathbb{R}_{+}\right)\right\} , \qquad (5)$$

it is the adjoint of the so-called initial symmetric operator \hat{H} associated with \check{H} and defined on the dense domain $D_H = \mathcal{D}(\mathbb{R}_+)$, the space of smooth functions with a compact support,

$$\mathcal{D}(\mathbb{R}_{+}) = \{ \psi(x) : \psi \in C^{\infty}(\mathbb{R}_{+}), \text{ supp} \psi \subseteq [\alpha, \beta] \subset (0, \infty) \}$$
 (6)

it is evident that $\mathcal{D}\left(\mathbb{R}_{+}\right)\subset D_{\check{H}}^{*}(\mathbb{R}_{+})$ and $\hat{H}\subset \hat{H}^{+}$. The operator \hat{H}^{+} is generally not self-adjoint and even not symmetric; its quadratic asymmetry form is denoted by $\Delta_{H^{+}}$. All possible Hamiltonians associated with \check{H} are defined as s.a. restrictions of \hat{H}^{+} , which simultaneously are s.a. extensions of the symmetric \hat{H} , the restrictions to some subspaces (domains) belonging to $D_{\check{H}}^{*}\left(\mathbb{R}_{+}\right)$ and specified by some additional (asymptotic) s.a. boundary conditions on functions belonging to $D_{\check{H}}^{*}\left(\mathbb{R}_{+}\right)$ under which the asymmetry form $\Delta_{H^{+}}$ becomes trivial (vanishes); these domains are maximum subspaces in $D_{\check{H}}^{*}\left(\mathbb{R}_{+}\right)$ where the operator \hat{H}^{+} is symmetric² (see [12]). Our first aim is to describe all these Hamiltonians. The special case of $g_{1}=0$ corresponds to the Calogero potential and was already considered in [24], we therefore keep $g_{1}\neq0$ in what follows.

This paper is organized as follows. In sec. 2 we present and discuss some exact solutions of equation (4) and their asymptotics. In the following five sections, we construct all s.a. extensions of \hat{H} , and perform the corresponding

¹a.c. means absolutely continuous.

² Although the notions "s.a. extension of \hat{H}^+ " and "s.a. restriction of \hat{H} " are equivalent; it is more customary to speak about s.a. extensions; we use one or another of the equivalent notions where appropriate.

spectral analysis of the Hamiltonians for different ranges of the parameter g_2 . In secs. (3.1-3.4), we consider the case of $g_2 \neq 0$. The special case of $g_2 = 0$ is considered in sec. 3.5. In sec. 4, we highlight some remarks and possible applications of the obtained results.

2 Exact solutions and asymptotics

We first consider the Schrödinger equation (4). Introducing a new variable z and new functions $\phi_{\pm}(z)$ instead of the respective x and $\psi(x)$,

$$z = \lambda x, \ \lambda = 2\sqrt{-W} = 2\sqrt{|W|}e^{i(\varphi - \pi)/2}, \ \psi(x) = x^{1/2 \pm \mu}e^{-z/2}\phi_{\pm}(z) ,$$

$$\mu = \begin{cases} \sqrt{g_2 + 1/4}, \ g_2 \ge -1/4 \\ i\varkappa, \ \varkappa = \sqrt{|g_2| - 1/4}, \ g_2 < -1/4 \end{cases} , \tag{7}$$

we reduce eq. (4) to the confluent hypergeometric equations for $\phi_{\pm}(z)$,

$$zd_z^2\phi_{\pm}(z) + (\beta_{\pm} - z)d_z\phi_{\pm}(z) - \alpha_{\pm}\phi_{\pm}(z) = 0 ,$$

$$\alpha_{+} = 1/2 \pm \mu + g_1/\lambda, \ \beta_{+} = 1 \pm 2\mu ,$$
(8)

their solutions are the known confluent hypergeometric functions $\Phi(\alpha_{\pm}, \beta_{\pm}; z)$ and $\Psi(\alpha_{\pm}, \beta_{\pm}; z)$, see [18, 19].

Solutions $\psi(x)$ of eq. (4) are restored from solutions of eqs. (8) by transformation (7). In what follows, we use $u_1(x; W)$, $u_2(x; W)$, and $v_1(x; W)$ defined by

$$u_{1}(x; W) = x^{1/2+\mu} e^{-z/2} \Phi(\alpha_{+}, \beta_{+}; z) = u_{1}(x; W)|_{\lambda \to -\lambda} ,$$

$$u_{2}(x; W) = x^{1/2-\mu} e^{-z/2} \Phi(\alpha_{-}, \beta_{-}; z) = u_{2}(x; W)|_{\lambda \to -\lambda} = u_{1}(x; W)|_{\mu \to -\mu} ,$$

$$v_{1}(x; W) = \lambda^{2\mu} x^{1/2+\mu} e^{-z/2} \Psi(\alpha_{+}, \beta_{+}; z) = \lambda^{2\mu} \frac{\Gamma(-2\mu)}{\Gamma(\alpha_{-})} u_{1} + \frac{\Gamma(2\mu)}{\Gamma(\alpha_{+})} u_{2} .$$
(9)

The function u_2 is not defined for $\beta_- = -n$, or $\mu = (n+1)/2, n \in \mathbb{Z}_+$, in particular, for $\mu = 1/2$. For such μ , we replace u_2 by other solutions of eq. (4), they are considered in the subsequent sections.

The coefficients of the Taylor expansion of functions $u_1(x; W)/x^{1/2+\mu}$ and $u_2(x; W)/x^{1/2-\mu}$ with respect to x are polynomials in λ . Because these functions are even in λ , the coefficients are polynomials in W, whence it follows that $u_1(x; W)$ and $u_2(x; W)$ are entire functions in W at any point x except x = 0 for u_2 with $\mu > 1/2$.

If $g_2 \ge -1/4$ ($\mu \ge 0$), then $u_1(x; W)$ and $u_2(x; W)$ are real-entire functions of W. If $g_2 < -1/4$ ($\mu = i\varkappa$), then $u_2(x; E) = u_1(x; E)$.

The pairs u_1, u_2 with $\mu \neq 0$ and u_1, v_1 for $\text{Im } W \neq 0$ are the fundamental systems of solutions of eq. (4) because the respective Wronskians are

$$\operatorname{Wr}(u_1, u_2) = -2\mu, \ \operatorname{Wr}(u_1, v_1) = -\Gamma(\beta_+)/\Gamma(\alpha_+) \equiv -\omega(W) \ .$$
 (10)

The well-known asymptotics of the special functions Φ and Ψ , see e.g. [18], entering solutions (9) allows simply estimating the asymptotic behavior of the solutions at the origin, as $x \to 0$, and at infinity, as $x \to \infty$.

As $x \to 0$, we have

$$\begin{split} u_1(x;W) &= \kappa_0^{-1/2 - \mu} u_{1\mathrm{as}}(x) + O(x^{3/2 + \mu}), \\ u_2(x;W) &= \kappa_0^{-1/2 + \mu} u_{2\mathrm{as}}(x) + \left\{ \begin{array}{l} O(x^{5/2 - \mu}), \; -1/4 < g_2 < 3/4, \; g_2 \neq 0, \\ (0 < \mu < 1, \mu \neq 1/2) &, \\ O(x^{3/2}), \; g_2 < -1/4 \; (\mu = i\varkappa) \end{array} \right. \end{split}$$

and, if $\alpha_{+} \neq -n$, $\alpha_{-} \neq -m$, $n, m \in \mathbb{Z}_{+}$,

$$v_{1}(x;W) = \begin{cases} \frac{\Gamma(2\mu)}{\Gamma(\alpha_{+})} x^{1/2-\mu} (1+O(x)), & g_{2} \geq 3/4 \ (\mu \geq 1) \\ \lambda^{2\mu} \frac{\Gamma(-2\mu)}{\Gamma(\alpha_{-})} \kappa_{0}^{-1/2-\mu} u_{1as}(x) + \frac{\Gamma(2\mu)}{\Gamma(\alpha_{+})} \kappa_{0}^{-1/2+\mu} u_{2as}(x) + O(x^{3/2}), \\ -1/4 < g_{2} < 3/4, g_{2} \neq 0 \ (0 < \mu < 1, \mu \neq 1/2) \\ \lambda^{2i\varkappa} \frac{\Gamma(-2i\varkappa)}{\Gamma(\alpha_{-})} \kappa_{0}^{-1/2-i\varkappa} u_{1as}(x) + \frac{\Gamma(2i\varkappa)}{\Gamma(\alpha_{+})} \kappa_{0}^{-1/2+i\varkappa} u_{2as}(x) + O(x^{3/2}), \\ g_{2} < -1/4 \ (\mu = i\varkappa) \end{cases}$$

$$(12)$$

where

$$u_{1as}(x) = (\kappa_0 x)^{1/2 + \mu},$$

$$u_{2as}(x) = \begin{cases} (\kappa_0 x)^{1/2 - \mu} - \frac{g_1/\kappa_0}{2\mu - 1} (\kappa_0 x)^{3/2 - \mu}, & -1/4 < g_2 < 3/4, \ g_2 \neq 0, \\ (0 < \mu < 1, \mu \neq 1/2) & , \\ (\kappa_0 x)^{1/2 - i\varkappa}, \ g_2 < -1/4 \ (\mu = i\varkappa) \end{cases}$$
(13a)

and κ_0 is an arbitrary, but fixed, parameter of dimension of inverse length. As $x \to \infty$, Im W > 0, we have

$$u_1(x; W) = \frac{\Gamma(\beta_+)}{\Gamma(\alpha_+)} \lambda^{\alpha_+ - \beta_+} x^{g_1/\lambda} e^{z/2} (1 + O(x^{-1})) = O(x^a e^{|W|^{1/2} \sin(\varphi/2)}) ,$$

$$v_1(x; W) = \lambda^{-\alpha_-} x^{-g_1/\lambda} e^{-z/2} (1 + O(x^{-1})) = O(x^{-a} e^{-|W|^{1/2} \sin(\varphi/2)}) ,$$

$$a = 2^{-1} |W|^{-1/2} g_1 \sin(\varphi/2) .$$

The obtained asymptotics are sufficient to allow definite conclusions about the deficiency indices of the initial symmetric operator \hat{H} as functions of the parameters g_1, g_2 and thereby about a possible variety of its s.a. extensions. It is evident that for $\operatorname{Im} W > 0$ the function $u_1(x; W)$ exponentially increasing at infinity and is not square-integrable. The function $v_1(x; W)$ exponentially decreasing at infinity is not square-integrable at the origin for $g_2 \geq 3/4$ ($\mu \geq 1$), whereas for $g_2 < 3/4$, it is (moreover, for $g_2 < 3/4$, any solution of eq. (4) is square-integrable at the origin). Because for $\operatorname{Im} W > 0$, the functions u_1, v_1 form a fundamental system of eq. (4), this equation with $\operatorname{Im} W > 0$ has no

square-integrable solutions for $g_2 \geq 3/4$, whereas for $g_2 < 3/4$, there exists one square-integrable solution, $v_1(x; W)$. This means that the deficiency indices of the initial symmetric operator \hat{H} are equal to zero, $m_{\pm} = 0$, for $g_2 \geq 3/4$ and are equal to unity, $m_{\pm} = 1$, for $g_2 < 3/4$.

Correspondingly for $g_2 \geq 3/4$, there is a unique s.a. extension of \hat{H} , whereas for $g_2 < 3/4$, there exists a one-parameter family of s.a. extensions of \hat{H} . A structure of these extensions, in particular, an appearance of their specifying asymptotic boundary conditions, depends crucially on a specific range of values of the parameter g_2 . In what follows, we distinguish five such regions and consider them separately.

3 Self-adjoint extensions and spectral analysis

3.1 The first range $g_2 \ge 3/4 \ (\mu \ge 1)$

As was mentioned above, the deficiency indices of the initial symmetric operator \hat{H} with g_2 in this range are zero. This implies that for $g_2 \geq 3/4$, the operator \hat{H}^+ is s.a. and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of \hat{H} with the domain $D_{H_{\epsilon}} = D_{\hat{H}}^*(\mathbb{R}_+)$ (5).

A spectral analysis of the s.a. operator $\hat{H}_1 = \hat{H}^+$ begins with an evaluation of its Green function G(x, y; W) that is the kernel of the integral representation of the solution $\psi_*(x)$ of the inhomogeneous differential equation

$$\left(\check{H} - W\right)\psi_*\left(x\right) = \eta(x), \, \eta(x) \in L^2(\mathbb{R}_+) \tag{14}$$

with Im $W \neq 0$ under the condition that $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$, i.e., that ψ_* is square-integrable³, $\psi_*(x) \in L^2(\mathbb{R}_+)$ (see [24, 25]). The general solution of this equation without the condition of square integrability can be represented as

$$\psi_*(x) = a_1 u_1(x; W) + a_2 v_1(x; W) + I(x; W) ,$$

$$\psi_*'(x) = a_1 u_1'(x; W) + a_2 v_1'(x; W) + I'(x; W) ,$$
 (15)

where

$$\begin{split} I(x;W) &= \int_0^x G^{(+)}\left(x,y;W\right)\eta(y)dy + \int_x^\infty G^{(-)}\left(x,y;W\right)\eta(y)dy \;, \\ I'(x;W) &= \int_0^x d_x G^{(+)}\left(x,y;W\right)\eta(y)dy + \int_x^\infty d_x G^{(-)}\left(x,y;W\right)\eta(y)dy \;, \\ G^{(+)}\left(x,y;W\right) &= \omega^{-1}(W)\upsilon_1(x;W)\upsilon_1(y;W) \;, \\ G^{(-)}\left(x,y;W\right) &= \omega^{-1}(W)\upsilon_1(x;W)\upsilon_1(y;W) \;, \end{split}$$

with ω given in (10). Using the Cauchy-Bunyakovskii inequality, it is easy to show that I(x; W) is bounded as $x \to \infty$. The condition $\psi_*(x) \in L^2(\mathbb{R}_+)$

³We note, that $D_{\check{H}}^*(\mathbb{R}_+)$ can be considered as the space of unique square-integrable solutions of eq. (14) with Im $W \neq 0$ and any $\eta(x) \in L^2(\mathbb{R}_+)$.

then implies that $a_1=0$, because $u_1(x;W)$ exponentially grows while $v_1(x;W)$ exponentially decreases at infinity. As $x\to 0$, we have $I(x)\sim O(x^{3/2})$, $I'(x)\sim O(x^{1/2})$ (up to the logarithmic accuracy at $g_2=3/4$), whereas $v_1(x;W)$ is not square-integrable at the origin. The condition $\psi_*(x)\in L^2(\mathbb{R}_+)$ then implies that $a_2=0$. In addition, we see that the asymptotic behavior of functions $\psi_*(x)$ belonging to $D_{\check{H}}^*(\mathbb{R}_+)$ at the origin, as $x\to 0$, is estimated by

$$\psi_*(x) = O(x^{3/2}), \ \psi_*'(x) = O(x^{1/2}).$$
 (16)

Together with the fact that the functions ψ_* vanish at infinity (see below), this implies that the asymmetry form Δ_{H^+} is trivial, which confirms that in the first range the operator \hat{H}^+ is symmetric and therefore self-adjoint (in contrast to the next ranges considered in the subsequent sections).

It follows that the Green's function is given by

$$G\left(x,y;W\right) = \left\{ \begin{array}{l} G^{(+)}\left(x,y;W\right), \ x > y \\ G^{(-)}\left(x,y;W\right), \ x < y \end{array} \right. .$$

The representation (9) of the function v_1 in terms of the functions u_1 and u_2 is inconvenient sometimes, because the individual summands do not exist for some μ although v_1 does. For our purposes, another representations are convenient. For $m-1 < 2\mu < m+1$, $m \geq 2$, the function $v_1(x;W)$ can be represented as

$$v_{1}(x; W) = A_{m}(W)u_{1}(x; W) + \frac{\omega(W)}{2\mu}v_{(m)}(x; W) ,$$

$$A_{m}(W) = \lambda^{2\mu} \frac{\Gamma(-2\mu)}{\Gamma(\alpha_{-})} + a_{m}(W) \frac{\Gamma(2\mu)\Gamma(\beta_{-})}{\Gamma(\alpha_{+})} ,$$

$$v_{(m)}(x; W) = u_{2}(x; W) - a_{m}(W)\Gamma(\beta_{-})u_{1}(x; W) ,$$

$$a_{m}(W) = \lambda^{m} \frac{\Gamma(\alpha_{+m})}{m!\Gamma(\alpha_{-m})}, \ \alpha_{\pm m} = \frac{1 \pm m}{2} + g_{1}/\lambda .$$

It is easy to see that all the coefficients $a_m(W)$ are polynomials in W which are real for Im W = 0 (W = E). In view of the relation

$$\lim_{\beta \to -n}^{-1} \Gamma(\beta) \Phi(\alpha, \beta; x) = \frac{x^{n+1} \Gamma(\alpha + n + 1)}{(n+1)! \Gamma(\alpha)} \Phi(\alpha + n + 1, n + 2; x)$$

(see [19, 18]), the functions $v_{(m)}(x; W)$ and $A_m(W)$ exist for $m-1 < 2\mu < m+1$ and for any W. In fact, $v_{(m)}(x; W)$ are particular solutions of eq. (4) which are real-entire in W and have the properties (for $m-1 < 2\mu < m+1$)

$$\operatorname{Wr}(u_1, v_{(m)}) = -2\mu, \ v_{(m)}(x; W) = x^{1/2-\mu}(1 + O(x)), \ x \to 0.$$

As a guiding functional, we take

$$\Phi(\xi;W) = \int_0^\infty U(x;W)\xi(x)dx, \ \xi \in \mathbb{D} = D_r(\mathbb{R}_+) \cap D_{H_\epsilon} \ , \tag{17}$$

where $U(x; W) = u_1(x; W)$ and $D_r(\mathbb{R}_+)$ is the space of arbitrary functions with a support bounded from the right: $\varphi(x) \in D_r(\mathbb{R}_+) \Longrightarrow \sup \varphi \subseteq [0, \beta], \beta < \infty$; the domain \mathbb{D} is dense in $L^2(\mathbb{R}_+)$. The functional $\Phi(\xi; W)$ (17) is a simple guiding functional, i.e., it satisfies the properties: 1) for a fixed ξ , the functional $\Phi(\xi; W)$ is an entire function of W; 2) if $\Phi(\xi_0; E_0) = 0$, Im $E_0 = 0$, $\xi_0 \in \mathbb{D}$, then the inhomogeneous equation $(\check{H} - E_0)\psi = \xi_0$ has a solution $\psi \in \mathbb{D}$; 3) $\Phi(\check{H}\xi; W) = W\Phi(\xi; W)$. It is easy to verify the properties 1) and 3), and it remains to verify that the property 2) also holds. Let

$$\Phi(\xi_0; E_0) = \int_0^b u_1(x; E_0) \xi_0(x) dx = 0, \ \xi_0 \in \mathbb{D}, \ \text{supp} \xi_0 \in [0, b] \ . \tag{18}$$

We consider the function $\psi(x)$ defined by

$$\psi(x) = \frac{1}{2\mu} \left[u_1(x; E_0) \int_x^b v_{(m)}(y; E_0) \xi_0(y) dy + v_{(m)}(x; E_0) \int_0^x u_1(y; E_0) \xi_0(y) dy \right]$$
(19)

that evidently satisfying the equation $(\check{H} - E_0)\psi(x) = \xi_0(x)$. Using condition (18), we obtain that $\operatorname{supp}\psi \in [0, b]$, i.e., $\psi \in D_r(\mathbb{R}_+)$, and therefore, $\psi \in L^2(c, b)$ for any c > 0. With taking the asymptotic behavior of functions $u_1(x; E_0)$, $v_{(m)}(x; E_0)$, and $\xi_0(x)$ at the origin into account, a simple evaluation of the integrals in representation (19) gives:

$$\psi(x) = \begin{cases} O(x^{1/2+\mu}), & 1 \le \mu < 3 \\ O(x^{7/2} \ln \delta), & \mu = 3 \\ O(x^{7/2}), & \mu > 3 \end{cases}, x \to 0,$$

i.e., $\psi \in D_{H_{\epsilon}}$, and therefore, $\psi \in \mathbb{D}$.

The derivative of the spectral function is given by

$$\sigma'(E) = \pi^{-1} \operatorname{Im} \left[\omega^{-1}(E+i0) A_m(E+i0) \right] .$$
 (20)

Because $\omega^{-1}(W)A_m(W)$ is an analytic function of μ , its value at $\mu = m/2$ is a limit as $\mu \to m/2$. For $\mu \neq m/2$, representation (20) can be simplified to

$$\sigma'(E) = \operatorname{Im} \Omega(E + i0), \ \Omega(W) = \frac{\lambda^{2\mu} \Gamma(-2\mu) \Gamma(\alpha_+)}{\pi \Gamma(\alpha_-) \Gamma(\beta_+)}.$$

For $E = p^2 \ge 0$, $p \ge 0$, $\lambda = 2pe^{-i\pi/2}$, we find

$$\sigma'(E) = \left(\frac{|\Gamma(\alpha_+)|}{\Gamma(\beta_+)}\right)^2 \frac{(2p)^{2\mu} e^{-\pi g_1/2p}}{2\pi} > 0.$$
 (21)

We see that $\sigma'(E)$ is a nonsingular function for $E \geq 0$. It follows that the spectrum of the s.a. Hamiltonian \hat{H}_1 is continuous for all such values of E.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\Omega(E)$ is real for all values of E where $\Omega(E)$ is finite, which implies that Im $\Omega(E + i0)$ can differ from zero

only at the discrete points E_n where $1/\Omega(E_n) = 0$. It is easy to see that the latter equation is reduced to the equations $\alpha_+(E_n) = -n, n \in \mathbb{Z}_+$, which have solutions only if $g_1 < 0$, and the solutions E_n are then given by

$$E_n = -g_1^2 (1 + 2\mu + 2n)^{-2}, \ \tau_n = |g_1| (1 + 2\mu + 2n)^{-1}.$$
 (22)

We thus obtain that for E < 0, the function $\sigma'(E)$ is equal to zero if $g_1 > 0$, whereas if $g_1 < 0$, this function is given by

$$\sigma'(E) = \sum_{n=0}^{\infty} Q_n^2 \delta(E - E_n) , \ Q_n = \frac{(2\tau_n)^{\mu+1}}{\Gamma(\beta_+)} \sqrt{\frac{\tau_n \Gamma(1 + 2\mu + n)}{|g_1| n!}} .$$

The final result of this section is as follows.

For $g_2 > 3/4$ ($\mu > 1$), the spectrum of a unique s.a. operator (Hamiltonian) \hat{H}_1 is simple and given by

$$\operatorname{spec} \hat{H}_1 = \begin{cases} \mathbb{R}_+, \ g_1 > 0 \\ \mathbb{R}_+ \cup \{E_n, \}, \ g_1 < 0 \end{cases}.$$

For $g_1 > 0$, its generalized eigenfunctions $U_E(x) = \sqrt{\sigma'(E)}u_1(x; E)$, $E \ge 0$, form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. For $g_1 < 0$, the generalized eigenfunctions $U_E(x) = \sqrt{\sigma'(E)}u_1(x; E)$, $E \ge 0$, of the continuous spectrum and the eigenfunctions $U_n(x) = Q_n u_1(x; E_n)$, $n \in \mathbb{Z}_+$, of the discrete spectrum form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

3.2 The second range $3/4 > g_2 > -1/4$, $g_2 \neq 0$ $(1 > \mu > 0, \ \mu \neq 1/2)$

We note that in this section, we consider the range $3/4 > g_2 > -1/4$ excluding the point $g_2 = 0$ ($\mu = 1/2$), the reason is that the function u_2 we use here is not defined for $\mu = 1/2$. The case $g_2 = 0$ ($\mu = 1/2$) is considered separately in the last subsection.

The operator \hat{H}^+ with g_2 in the second range is not s.a., and we must construct its s.a. reductions. In accordance with the general procedure of the alternative method, see [12] and also [24], [25] for examples, we begin with evaluating the quadratic asymmetry form Δ_{H^+} in terms of quadratic boundary forms, which are determined by the asymptotics of functions $\psi_*(x)$ belonging to the natural domain $D_{\check{H}}^*(\mathbb{R}_+)$ at the origin (the left boundary form) and at infinity (the right boundary form). Because the potential vanishes at infinity, the right boundary form is trivial (zero)⁴, see [12], and the asymmetry form Δ_{H^+} is reduced to (minus) the left boundary form. To determine an asymptotic behavior of functions ψ_* at the origin, we consider these functions as solutions of the inhomogeneous eq. (14) with W = 0. Because in the range under

⁴Moreover, we can prove that ψ_* vanishes at infinity together with its derivative, $\psi_*(x), \psi_*'(x) \stackrel{x \to \infty}{\longrightarrow} 0$.

consideration, any solution of the homogeneous eq. (4) is square-integrable at the origin, the general solution of eq. (14) with W = 0 can be represented as

$$\psi_*(x) = a_1 u_1(x;0) + a_2 u_2(x;0) - \frac{1}{2\mu} \int_0^x \left[u_1(x;0) u_2(y;0) - u_2(x;0) u_1(y;0) \right] \eta(y) dy .$$
 (23)

The asymptotic behavior of the functions u_1 and u_2 in representation (23) as $x \to 0$ is given by (11) and (13a), the asymptotic behavior of the integral terms is estimated using the Cauchy-Bunyakovskii inequality, and we find

$$\psi_*(x) = a_1 u_{1as}(x) + a_2 u_{2as}(x) + O(x^{3/2}) ,$$

$$\psi_*'(x) = a_1 u_{1as}'(x) + a_2 u_{2as}'(x) + O(x^{1/2}) .$$
 (24)

With these asymptotics, we calculate the left boundary form $[\psi_*, \psi_*](0) = \lim_{x\to 0} (-\overline{\psi}_*(x)\psi'_*(x)+\overline{\psi}'_*(x)\psi_*(x))$ and obtain a representation of the quadratic asymmetry form as a quadratic form in the coefficients a_1 and a_2 in (24):

$$\Delta_{H^+}(\psi_*) = -2\mu k_0(\overline{a_1}a_2 - \overline{a_2}a_1) .$$

The coefficients a_1, a_2 are called the (left) asymptotic boundary (a.b.) coefficients⁵. The requirement on the a.b. coefficients that Δ_{H^+} vanish results in the relation⁶

$$a_2 \sin \nu = a_1 \cos \nu \ , \ \nu \in \mathbb{S}(-\pi/2, \pi/2) \ ,$$
 (25)

between these coefficients. It follows that the quadratic asymmetry form Δ_{H^+} becomes trivial on the subspaces of $D^*_{\tilde{H}}$ such that the a.b. coefficients of functions $\psi_*(x)$ belonging to $D^*_{\tilde{H}}$ satisfy relation (25) with fixed ν . These subspaces are just the domains of s.a. restrictions of \hat{H}^+ , and relation (25), with fixed ν , defines the asymptotic boundary conditions specifying these s.a. operators.

We thus obtain that for each g_2 in the second range, there exists a family of s.a. Hamiltonians $\hat{H}_{2,\nu}$ parametrized by the parameter ν on a circle with the domains $D_{H_{2\nu}}$ that are the subspaces of functions belonging to $D_{\check{H}}^*(\mathbb{R}_+)$ and having the following asymptotic behavior at the origin, as $x \to 0$,

$$\psi(x) = C\psi^{as}(x) + O(x^{3/2}) , \ \psi'(x) = C\psi^{as\prime}(x) + O(x^{1/2}) ,$$

$$\psi^{as}(x) = u_{1as}(k_0 x) \sin \nu + u_{2as}(x, k_0) \cos \nu .$$
 (26)

The spectral analysis of $\hat{H}_{2,\nu}$ is similar to that for \hat{H}_1 in the previous section, the difference is that the function $v_1(x;W)$ is now square-integrable at the origin and we must take asymptotic boundary conditions (26) into account. To evaluate the Green's function for $\hat{H}_{2,\nu}$, we take the representation (15) with

⁵ The inertia indices of the quadratic form $(1/2i\mu\kappa_0)\Delta_+$ are 1, 1, which confirms the previos assertion in sec. (2) that the deficiency indices of \hat{H} are $m_+ = 1$, see [12].

⁶Here and in what follows we use the notation $\mathbb{S}(a,b) = [a,b]$, $a \sim b$.

 $a_1 = 0$ for $\psi_*(x)$ belonging to $D_{H_{2\nu}}$, boundary conditions (26), and asymptotics (11), (13a) then yield

$$a_2 = k_0^{-2\mu} \omega^{-1}(W) \left[\frac{\Gamma(2\mu)}{\Gamma(\alpha_+)} \sin \nu - \frac{\Gamma(-2\mu)(\lambda/k_0)^{2\mu}}{\Gamma(\alpha_-)} \cos \nu \right]^{-1} \times \cos \nu \int_0^\infty \upsilon_1(x; W) \eta(x) dx .$$

Representing the function $v_1(x; W)$ in the form

$$\begin{split} v_1(x;W) &= (2\mu)^{-1} k_0^{-1/2} \lambda^{\mu} [\tilde{\omega}_{2,\nu}(W) u_{2,\nu}(x;W) + \omega_{2,\nu}(W) \tilde{u}_{2,\nu}(x;W)] \;, \\ u_{2,\nu}(x;W) &= k_0^{1/2+\mu} u_1(x;W) \sin \nu + k_0^{1/2-\mu} u_2(x;W) \cos \nu \;, \\ \tilde{u}_{2,\nu}(x;W) &= -k_0^{1/2+\mu} u_1(x;W) \cos \nu + k_0^{1/2-\mu} u_2(x;W) \sin \nu \;, \\ \omega_{2,\nu}(W) &= \omega(W) (\lambda/k_0)^{-\mu} \sin \nu + (\lambda/k_0)^{\mu} \frac{\Gamma(\beta_-)}{\Gamma(\alpha_-)} \cos \nu \;, \\ \tilde{\omega}_{2,\nu}(W) &= \omega(W) (\lambda/k_0)^{-\mu} \cos \nu - (\lambda/k_0)^{\mu} \frac{\Gamma(\beta_-)}{\Gamma(\alpha_-)} \sin \nu \;, \end{split}$$

where ω is given in (10), the functions $u_{2,\nu}(x;W)$ and $\tilde{u}_{2,\nu}(x;W)$ are real-entire in W solutions of eq. (4) and $u_{2,\nu}(x;W)$ satisfies boundary condition (26), we obtain the Green function

$$G(x, y; W) = (2\mu k_0)^{-1} \Omega(W) u_{2,\nu}(x; W) u_{2,\nu}(y; W) + \frac{1}{2\mu k_0} \begin{cases} \tilde{u}_{2,\nu}(x; W) u_{2,\nu}(y; W), & x > y \\ u_{2,\nu}(x; W) \tilde{u}_{2,\nu}(y; W), & x < y \end{cases},$$
(27)

where

$$\Omega(W) = \omega_{2,\nu}^{-1}(W)\tilde{\omega}_{2,\nu}(W)$$
 (28)

We note that the second summand in (27) is real for real W = E.

As a guiding functional we take the functional $\Phi(\xi; W)$ given by (17) with $U(x; W) = u_{2,\nu}(x; W)$ and $\xi \in \mathbb{D} = D_r(\mathbb{R}_+) \cap D_{H_{2,\nu}}$. The domain \mathbb{D} is dense in $L^2(\mathbb{R}_+)$, $\overline{\mathbb{D}} = L^2(\mathbb{R}_+)$. Following the procedure of the previous section, we show that $\Phi(\xi; z)$ is a simple guiding functional, i.e., satisfies the properties 1)-3) cited in subsec. 3.1. It is easy to verify the properties 1) and 3). We prove that the property 2) also holds. Let

$$\Phi(\xi_0; E_0) = \int_0^b u_{2,\nu}(x; E_0) \xi_0(x) dx = 0, \ \xi_0 \in \mathbb{D}, \ \text{supp} \xi_0 \in [0, b] \ . \tag{29}$$

We consider the function

$$\psi(x) = \frac{1}{2\mu\kappa_0} \left[u_{2,\nu}(x; E_0) \int_x^b \tilde{u}_{2,\nu}(y; E_0) \xi_0(y) dy + \tilde{u}_{2,\nu}(x; E_0) \int_0^x u_{2,\nu}(y; E_0) \xi_0(y) dy \right],$$

which is a solution of equation

$$(\check{H} - E_0)\psi(x) = \xi_0(x)$$
.

Using condition (29), we obtain that $\operatorname{supp} \psi \in [0, b]$, i.e., $\psi \in D_r(\mathbb{R}_+)$, and therefore $\psi \in L^2(c, b)$ for any c > 0.

The function $\psi(x)$ allows the representation

$$\psi(x) = cu_{2,\nu}(x; E_0) + \tilde{u}_{2,\nu}(x; E_0) \int_0^x u_{2,\nu}(y; E_0) \xi_0(y) dy$$
$$- u_{2,\nu}(x; E_0) \int_0^x \tilde{u}_{2,\nu}(y; E_0) \xi_0(y) dy, \ c = \frac{1}{2\mu\kappa_0} \int_0^b \tilde{u}_{2,\nu}(y; E_0) \xi_0(y) dy \ . \tag{30}$$

Using the asymptotics of functions $u_{2,\nu}(x; E_0)$, $\tilde{u}_{2,\nu}(x; E_0)$, and $\xi_0(x)$ and simple estimates of the asymptotic behavior of the integral terms at the origin, we obtain that the asymptotic of $\psi(x)$ at the origin is given by

$$\psi(x) = cu_{2,\nu}(x; E_0) + O(x^{5/2-\mu}), x \to 0$$

which implies that $\psi \in D_{H_{2,\nu}}$ and therefore $\psi \in \mathbb{D}$.

The derivative of the spectral function reads

$$\sigma'(E) = (2\pi\mu k_0)^{-1} \operatorname{Im} \Omega(E+i0)$$
.

It is convenient to consider the cases $|\nu| < \pi/2$ and $\nu = \pm \pi/2$ separately. We first consider the case $\nu = \pi/2$ where we have

$$u_{2,\pi/2}(x;W) = k_0^{1/2+\mu} u_1(x;W),$$

$$\sigma'(E) = \operatorname{Im} \Omega(E+i0), \ \Omega(W) = -\frac{\Gamma(\beta_-)\Gamma(\alpha_+)(\lambda/k_0)^{2\mu}}{2\pi\mu k_0\Gamma(\beta_+)\Gamma(\alpha_-)} \ .$$

For $E = p^2 \ge 0$, $p \ge 0$, $\lambda = 2pe^{-i\pi/2}$, we have

$$\sigma'(E) = \frac{|\Gamma(\alpha_+)|^2}{\Gamma^2(\beta_+)} \frac{(2p/k_0)^{2\mu} \mathrm{e}^{-\pi g_1/2p}}{2\pi k_0} \ ,$$

such that $\sigma'(E)$ is finite and $\operatorname{spec} H_{2,\pi/2} = \mathbb{R}_+$.

For $E=-\tau^2<0$, $\tau>0$, $\lambda=2\tau$, the function $\Omega(E)$ is real for all values of E where $\Omega(E)$ is finite, which implies that $\operatorname{Im}\Omega(E+i0)$ can differ from zero only at the discrete points E_n where $1/\Omega(E_n)=0$. The latter equation is reduced to the equations $\alpha_-(E_n)=-n, n\in\mathbb{Z}_+$, $(\Gamma(\alpha_+)=\infty)$ or

$$1 + 2\mu + g_1/\tau_n = -2n, \ n \in \mathbb{Z}_+ \ . \tag{31}$$

Eqs. (31) have no solutions for $g_1 > 0$ and for $g_1 < 0$ we have (we will denote the points of discrete spectrum for $\nu = \pm \pi/2$ by \mathcal{E}_n)

$$\tau_n = \frac{|g_1|}{1 + 2\mu + 2n}, \ \mathcal{E}_n = -\tau_n^2 = -\frac{g_1^2}{(1 + 2\mu + 2n)^2},$$

such that we obtain

$$\sigma'(E) = \sum_{n=0}^{\infty} Q_n^2 \delta(E - \mathcal{E}_n) , \ Q_n = \frac{(2\tau_n)^{\mu+1} k_0^{-(1/2+\mu)}}{\Gamma(\beta_+)} \sqrt{\frac{\Gamma(1+2\mu+n)}{(1+2\mu+2n) n!}}$$

It is easy to see that for the case of $\nu = -\pi/2$, we obtain the same results for spectrum and eigenfunctions as it must be.

The final result for the Hamiltonian $\hat{H}_{2,\pm\pi/2}$ is as follows. Its spectrum is simple and given by

$$\mathrm{spec} \hat{H}_{2,\pm\pi/2} = \left\{ \begin{array}{l} \mathbb{R}_+, \ g_1 > 0 \ , \\ \mathbb{R}_+ \cup \{\mathcal{E}_n, \ n \in \mathbb{Z}_+\}, \ g_1 < 0 \end{array} \right.,$$

and the complete orthonormalized system of its eigenfunctions in $L^2(\mathbb{R}_+)$ is given by

$$U_{E}(x) = \sqrt{\sigma'(E)} k_{0}^{1/2+\mu} u_{1}(x; E), E \ge 0,$$

$$U_{n}(x) = \frac{2^{1-\mu} |\mathcal{E}_{n}|^{3/4-\mu/2}}{|g_{1}|^{1/2} |\Gamma(\beta_{-})|} \sqrt{q_{n}} u_{2}(x; \mathcal{E}_{n}),$$

$$q_{n} = \begin{cases} \Gamma^{-1}(1+n)\Gamma(1+n-2\mu), 0 < \mu < 1/2 \\ \Gamma^{-1}(2+n)\Gamma(2+n-2\mu), 1/2 < \mu < 1 \end{cases}, n \in \mathbb{Z}_{+},$$

for $g_1 > 0$, and by

$$U_{E}(x) = \sqrt{\sigma'(E)} k_0^{1/2+\mu} u_1(x; E), \ E \ge 0 ,$$

$$U_{n}(x) = Q_{n} k_0^{1/2+\mu} u_1(x; \mathcal{E}_n) ,$$

for $q_1 < 0$.

Now, we turn to the case $|\nu| < \pi/2$. In this case we have

$$\sigma'(E) = (2\pi\mu k_0 \cos^2 \nu)^{-1} \operatorname{Im} F_{2,\nu}^{-1}(E+i0) ,$$

$$F_{2,\nu}(W) = f_2(W) + \tan \nu, \ f_2(W) = \frac{\Gamma(\beta_-)\Gamma(\alpha_+)(\lambda/k_0)^{2\mu}}{\Gamma(\beta)\Gamma(\alpha_-)} .$$

For $E = p^2 \ge 0$, $p \ge 0$, $\lambda = 2pe^{-i\pi/2}$, we have

$$\sigma'(E) = \frac{B(E)}{2\pi k_0 \cos^2 \nu [A^2(E) + \mu^2 B^2(E)]} , \qquad (32)$$

where $A(E) = \operatorname{Re} F_{2,\nu}(E)$ and $\mu B(E) = -\operatorname{Im} F_{2,\nu}(E)$. A direct calculation gives

$$A(E) = \frac{\mu |\Gamma(\alpha_{+})|^{2} (2p/k_{0})^{2\mu}}{\Gamma^{2}(\beta_{+}) \sin(2\pi\mu)} \left(e^{-\pi g_{1}/2p} \cos(2\pi\mu) + e^{\pi g_{1}/2p} \right) + \tan \nu ,$$

$$B(E) = \frac{|\Gamma(\alpha_{+})|^{2} (2p/k_{0})^{2\mu} e^{-\pi g_{1}/2p}}{\Gamma^{2}(\beta)} > 0 .$$
(33)

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $F_{2,\nu}(E)$ is real, therefore, $\sigma'(E)$ can differ from zero only at the discrete points $E_n(\nu)$ such that $F_{2,\nu}(E_n(\nu)) = 0$, or $f_2(E_n(\nu)) = -\tan \nu$, and we obtain that (derivatives with respect to E are denoted by primes in eq. (34))

$$\sigma'(E) = \sum_{n} \left[-2\mu k_0 F'_{2,\nu}(E_n(\nu)) \cos^2 \nu \right]^{-1} \delta(E - E_n(\nu)) ,$$

$$F'_{2,\nu}(E_n(\nu)) = f'_2(E_n(\nu)) < 0, \ \partial_{\nu} E_n(\nu) = -\cos^{-2}\nu \left[f'_2(E_n(\nu))\right]^{-1} > 0.$$
 (34)

I. Let $g_1 > 0$

For $E = p^2 > 0$, p > 0, the function $\sigma'(E)$ (32) is a finite positive function. At E = 0, we have B(0) = 0 and

$$A(0)|_{\nu=\nu_0} = 0$$
, $\tan \nu_0 = -\Gamma(\beta_-)(g_1/k_0)^{2\mu}\Gamma^{-1}(\beta_+)$.

It is easy to see that

$$F_{2,\nu}(W) = \tan \nu - \tan \nu_0 - \left(2\mu k_0 \cos^2 \nu_0\right)^{-1} \Psi^{-2}W + O(W), \ W \to 0 ,$$

$$\Psi = \frac{g_1(g_1/k_0)^{-\mu}}{\mu \cos \nu_0} \sqrt{\frac{3\Gamma(1+2\mu)}{2k_0(1+2\mu)\Gamma(2-2\mu)}} .$$

It follows that for $\nu \neq \nu_0$, the function $\sigma'(E)$ is finite at E=0. But for $\nu=\nu_0$ and for small E, we have:

$$\sigma'(E) = -\frac{1}{\pi} \Psi^2 \operatorname{Im} (E + i0)^{-1} + O(1) = \Psi^2 \delta(E) + O(1) ,$$

which means that there is the eigenvalue E=0 in the spectrum of the s.a. Hamiltonian \hat{H}_{2,ν_0} . For $E = -\tau^2 < 0$, $\lambda = 2\tau$, the function $f_2(E)$,

$$f_2(E) = \frac{\Gamma(\beta_-)}{\Gamma(\beta_+)} \frac{\Gamma(1/2 + \mu + g_1/2\tau)(2\tau/k_0)^{2\mu}}{\Gamma(1/2 - \mu + g_1/2\tau)} ,$$

has the properties: $f_2(E)$ is smooth function for $E \in (-\infty,0), f_2(E) \to \infty$ as $E=-\infty, f_2(0)=-\tan\nu_0$. Because $f_2'(E_{\nu|n})<0$, see eq. (34), the straight line $f(E) = 2\mu \tan \nu, E \in (-\infty, 0]$, can intersect the plot of the function $f_2(E)$ no more than once.

That is why the equation $F_{2,\nu}(E) = 0$ has no solutions for $\nu \in (\nu_0, \pi/2)$ while for any fixed $\nu \in (-\pi/2, \nu_0]$, this equation has only one solution $E^{(-)}(\nu) \in$ $(-\infty, 0]$, which increases monotonically from $-\infty$ to 0 as ν changes from $-\pi/2+$ 0 to ν_0 .

We thus obtain that the spectrum of $H_{2,\nu}$, $|\nu| < \pi/2$, with $g_1 > 0$ is simple and given by

$$\operatorname{spec}\hat{H}_{2,\nu} = \begin{cases} \mathbb{R}_{+} \cup \{E^{(-)}(\nu)\}, \ \nu \in (-\pi/2, \nu_{0}] \\ \mathbb{R}_{+}, \ \nu \in (\nu_{0}, \pi/2) \text{ or } \nu = \pm \pi/2 \end{cases}$$
 (35)

The generalized eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} u_{2,\nu}(x; E), E \ge 0$$
,

and (for $\nu \in (-\pi/2, \nu_0]$) the eigenfunction

$$U_n(x) = U(x) = \left[-2\mu k_0 F'_{2,\nu}(E^{(-)}(\nu)) \cos^2 \nu \right]^{-1/2} u_{2,\nu} \left(x; E^{(-)}(\nu) \right)$$

of $\hat{H}_{2,\nu}$, form a complete orthonormalized systems in $L^2(\mathbb{R}_+)$.

II. Let $g_1 < 0$. Then:

For $E = p^2 \ge 0$, $p \ge 0$, $\lambda = 2pe^{-i\pi/2}$, formulas (32) and (33) hold true. Because the functions A(E) and B(E) are finite at E=0 ($B(0)\neq 0$), the function $\sigma'(E)$ (32) is a finite positive function for $E \geq 0$. This means that for $E \geq 0$, the spectra of s.a. Hamiltonians $\hat{H}_{2,\nu}$ are simple, purely continuous, and given by $\operatorname{spec} \hat{H}_{2,\nu} = \mathbb{R}_+$. For $E = -\tau^2 < 0, \, \tau > 0, \, \lambda = 2\tau$, we have

$$f_2(E) = \frac{\Gamma(\beta_-)}{\Gamma(\beta_+)} \frac{\Gamma(1/2 + \mu - |g_1|/2\tau)(2\tau/k_0)^{2\mu}}{\Gamma(1/2 - \mu - |g_1|/2\tau)} .$$

It is easy to see that for fixed ν , the spectrum is bounded from below and the equation $F_{2,\nu}(E) = 0$ has infinite number of solutions

$$E_n(\nu) = -g_1^2/4n^2 + O(n^{-3}) , \qquad (36)$$

asymptotically coinciding with (22) as $n \to \infty$.

We thus obtain that the spectrum of $H_{2,\nu}$, $|\nu| < \pi/2$, with $g_1 < 0$ is simple and given by spec $H_{2,\nu} = \mathbb{R}_+ \cup \{E_n(\nu)\}$. The corresponding generalized eigenfunctions of the continuous spectrum

$$U_E(x) = \sqrt{\sigma'(E)} u_{2,\nu}(x; E), E \ge 0$$
,

and eigenfunctions of the discrete spectrum

$$U_n(x) = \left[-2\mu k_0 F'_{2,\nu}(E_n(\nu))\cos^2\nu\right]^{-1/2} u_{2,\nu}(x; E_n(\nu)), \ E_n(\nu) < 0 \ ,$$

of $\hat{H}_{2,\nu}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

It is possible to give a comparison description of the Hamiltonians $\hat{H}_{2,\nu}, |\nu| <$ $\pi/2$ in more detail.

The function $f_2(E)$ has the properties: $f_2(E) \to \infty$ as $E \to -\infty$; $f_2(\mathcal{E}_n \pm 0) =$ $\pm \infty$, $n \in \mathbb{Z}_+$. Taking the third equality in (34) into account, we can see that: in each energy interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n \in \mathbb{Z}_+$, for a fixed $\nu \in (-\pi/2, \pi/2)$, there are one discrete level $E_n(\nu)$ which increases monotonically from $\mathcal{E}_{n-1}+0$ to $\mathcal{E}_n - 0$ when ν changes from $\pi/2 - 0$ to $-\pi/2 + 0$ (we set $\mathcal{E}_{-1} = -\infty$). We note that the relations

$$\lim_{\nu \to \pi/2} E_n(\nu) = \lim_{\nu \to -\pi/2} E_{n+1}(\nu) = \mathcal{E}_n, \ n \in \mathbb{Z}_+,$$

confirm the equivalence of s.a. extensions with parameters $\nu = -\pi/2$ and $\nu = \pi/2$.

We note that it is possible to find the explicit expressions for spectrum, spectral function, and the complete orthonormalized system of (generalized) functions of the s.a. Hamiltonian for $\nu = 0$. In this case, results are the same as in the first range $(g_2 \geq 3/4)$ with additional change $\mu \to -\mu$. One can easily verify that such calculated spectrum coincide with the spectrum $\{E_n(0)\}$.

It should be also pointed out that bound states exist even for the repulsive potential, $g_2,g_1>0$, see the dashed line on the Figure 1.

3.3 The third range $g_2 = -1/4 \ (\mu = 0)$

The analysis in this section is similar to that in the previous one, a peculiarity is that $\alpha_{+} = \alpha_{-} = \alpha = 1/2 + g_1/\lambda$, $\beta_{+} = \beta_{-} = 1$, $u_1(x; W) = u_2(x; W)$, and representation (9) of $v_1(x; W)$ in terms of u_1 and u_2 does not hold. As the solutions of eq. (4) with $g_2 = -1/4$, we therefore use the functions $u_1(x; W)$, $u_3(x; W)$, and $v_1(x; W)$ respectively defined by

$$\begin{split} u_1\left(x;W\right) &= x^{1/2} \mathrm{e}^{-z/2} \Phi(\alpha,1;z) = \left. u_1\left(x;W\right) \right|_{\lambda \to -\lambda} \;, \\ u_3\left(x;W\right) &= x^{1/2} \mathrm{e}^{-z/2} \frac{\partial}{\partial \mu} \left[x^{\mu} \Phi(1/2 + \mu + g_1/\lambda, 1 + 2\mu; z) \right]_{\mu = 0} + u_1\left(x;W\right) \ln k_0 \;, \\ v_1\left(x;W\right) &= x^{1/2} \mathrm{e}^{-z/2} \Psi(\alpha,1;z) = \Gamma^{-1}(\alpha) \left[\omega_0(W) u_1^{(0)}\left(x;W\right) - u_3\left(x;W\right) \right] \;, \\ \omega_0(W) &= 2\psi(1) - \psi(\alpha) - \ln(\lambda/k_0), \quad \alpha = 1/2 + g_1/\lambda \;, \end{split}$$

where $\psi(\alpha) = \Gamma'(\alpha)/\Gamma(\alpha)$ and k_0 is a constant. The functions $u_1(x; W)$ and $u_3(x; W)$ are real entire in W.

The asymptotic behavior of these functions at the origin and at infinity is respectively as follows.

As
$$x \to 0$$
, $z = \lambda x \to 0$, we have

$$u_1(x;W) = k_0^{-1/2} u_{1as}(x) + O(x^{3/2}), \quad u_{1as}(x) = (k_0 x)^{1/2},$$

$$u_3(x;W) = k_0^{-1/2} u_{3as}(x) + O(x^{3/2} \ln x), \quad u_{3as}(x) = (k_0 x)^{1/2} \ln(k_0 x),$$

$$v_1(x;W) = k_0^{-1/2} \Gamma^{-1}(\alpha) \left[\omega_0(W) u_{1as}(x) - u_{3as}(x)\right] + O(x^{3/2} \ln x). \quad (37)$$

As $x \to \infty$, Im W > 0, we have

$$u_1(x; W) = \Gamma^{-1}(\alpha) \lambda^{\alpha - 1} x^{g_1/\lambda} e^{z/2} \left[1 + O(x^{-1}) \right] \to \infty ,$$

$$v_1(x; W) = \lambda^{-\alpha} x^{-g_1/\lambda} e^{-z/2} \left[1 + O(x^{-1}) \right] \to 0 .$$
 (38)

The functions u_1 and u_3 are linearly independent and form a fundamental system of solutions of eq. (4), as well as the functions u_1 and v_1 for Im $W \neq 0$, see sec. 2,

Wr
$$(u_1, u_3) = 1$$
, Wr $(u_1, v_1) = -\Gamma^{-1}(\alpha)$.

We recall that, for $g_2 = -1/4$, the deficiency indices of the initial symmetric operator \hat{H} are $m_{\pm} = 1$, and therefore there exists a one-parameter family of s.a. extensions of \hat{H} with $g_2 = -1/4$, see sec. 2.

To evaluate the asymmetry form in terms of a.b. coefficients, we need to determine the asymptotics of functions ψ_* belonging to the natural domain $D_{\tilde{H}}^*(\mathbb{R}_+)$ at the origin. To this end, we use representation (23) of the general solution of eq. (14) with W=0 where the natural substitutions $a_2u_2 \to a_2u_3$ and $u_2/2\mu \to -u_3$ must be made. Using the Cauchy-Bunyakovskii inequality for estimating the integral terms, we obtain that the desired asymptotic as $x \to 0$ is given by

$$\psi_*(x) = a_1 u_{1as}(x) + a_2 u_{3as}(x) + O(x^{3/2} \ln x) ,$$

$$\psi_*'(x) = a_1 u_{1as}'(x) + a_2 u_{3as}'(x) + O(x^{1/2} \ln x) ,$$

and we find⁷ $\Delta_{H^+}(\psi_*) = k_0(\overline{a_1}a_2 - \overline{a_2}a_1)$, the coefficients a_1, a_2 are just a.b. coefficients. The requirement that Δ_{H^+} vanish results in the relation

$$a_1 \cos \vartheta = a_2 \sin \vartheta, \ \vartheta \in \mathbb{S} \left(-\pi/2, \pi/2 \right) \ .$$

This relation with fixed ϑ defines the domain of a possible Hamiltonian as a s.a. restriction of \hat{H}^+ , or a s.a. extension of \hat{H} .

The final result is that: for $g_2=-1/4$, there exists a family of s.a. Hamiltonians $\hat{H}_{3,\vartheta}$ with the domains

$$D_{H_{3,\vartheta}} = \left\{ \psi : \psi \in D_{\check{H}}^*(\mathbb{R}_+), \ \psi \text{ satisfies (39)} \right\} \ ,$$

where (39) are the asymptotic s.a. boundary conditions at the origin

$$\psi = C\psi_{3,\vartheta_{as}}(x) + O(x^{3/2}\ln x), \ \psi' = C\psi'_{3,\vartheta_{as}}(x) + O(x^{1/2}\ln x) \ x \to 0 \ ,$$

$$\psi_{3,\vartheta_{as}}(x) = u_{1as}(x)\sin\vartheta + u_{3as}(x)\cos\vartheta \ . \tag{39}$$

To evaluate the Green's function G(x, y; W) for $\hat{H}_{3,\vartheta}$, we take the representation (15) with $a_1 = 0$ for $\psi_*(x)$ belonging to $D_{H_{3,\vartheta}} \subset D_{\check{H}}^*(\mathbb{R}_+)$, boundary conditions (39) and asymptotics (37) then yield

$$a_2 = -\Gamma^2(\alpha)\cos\vartheta \left[\omega_0(W)\cos\vartheta + \sin\vartheta\right]^{-1} \int_0^\infty v_1(x;W)\eta(x)dx .$$

Using the representation

$$\Gamma(\alpha)v_1 = (\omega_0 \sin \vartheta - \cos \vartheta)u_{3,\vartheta} + (\omega_0 \cos \vartheta + \sin \vartheta)\tilde{u}_{3,\vartheta} ,$$

$$u_{3,\vartheta}(x;W) = u_1(x;W)\sin \vartheta + u_3(x;W)\cos \vartheta ,$$

$$\tilde{u}_{3,\vartheta}(x;W) = u_1(x;W)\cos \vartheta - u_3(x;W)\sin \vartheta ,$$

This structure of Δ_{H^+} confirms the previos assertion that the deficiency indices of \hat{H} are $m_+=1$.

where $u_{3,\vartheta}$ and $\tilde{u}_{3,\vartheta}$ are solutions of eq. (4) real-entire in W, and $u_{3,\vartheta}$ satisfies boundary condition (39), we find

$$G(x, y; W) = \Omega(W)u_{3,\vartheta}(x; W)u_{3,\vartheta}(y; W) + \begin{cases} \tilde{u}_{3,\vartheta}(x; W)u_{3,\vartheta}(y; W), & x > y \\ u_{3,\vartheta}(x; W)\tilde{u}_{3,\vartheta}(y; W), & x < y \end{cases}, \Omega(W) = (\omega_0(W)\cos\vartheta + \sin\vartheta)^{-1}(\omega_0(W)\sin\vartheta - \cos\vartheta).$$
(40)

We note that the second summand in G(x, y; W) is real for real W = E.

It is easy to verify that the guiding functional given by (17) with $U = u_{3,\vartheta}$ satisfies the properties 1) and 3) cited in subsec. 3.1. The proof that it satisfies the property 2) is identical to that presented in subsec. 3.2 for the second range $1 > \mu > 0$. It follows that the spectra of $\hat{H}_{3,\vartheta}$ are simple.

The derivative of the spectral function is given by $\sigma'(E) = \pi^{-1} \operatorname{Im} [\Omega(E+i0)]$. We first consider the case $\vartheta = \pi/2$ where we have

$$u_{3,\pi/2}(x;W) = u_1(x;W)$$
,
 $\sigma'(E) = -\pi^{-1} \operatorname{Im} \Omega(E+i0), \ \Omega(W) = \psi(\alpha) + \ln(\lambda/k_0)$.

For $E = p^2 \ge 0$, $p \ge 0$, $\lambda = 2pe^{-i\pi/2}$, we find

$$\sigma'(E) = \frac{1}{2} \left(1 - \tanh \frac{\pi g_1}{2p} \right) \ge 0$$
.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, and $g_1 > 0$, the function $\Omega(E)$ is of the form

$$\Omega(E) = \psi(1/2 + g_1/2\tau) + \ln(2\tau/k_0)$$
,

which implies that for $g_1 > 0$, there is no negative part of the spectrum.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, and $g_1 < 0$, we have

$$\Omega(E) = \psi(1/2 - |g_1|/2\tau) + \ln(2\tau/k_0), \text{ Im } \Omega(E) = \text{Im } \psi(1/2 - |g_1|/2\tau),$$

which implies that there are discrete negative energy levels \mathcal{E}_n in the spectrum,

$$\mathcal{E}_n = -g_1^2 (1+2n)^{-2}, \ \tau_n = |g_1|(1+2n)^{-1}, \ n \in \mathbb{Z}_+$$
$$\sigma'(E) = \sum_{n \in \mathbb{Z}_+} Q_n^2 \delta(E - \mathcal{E}_n), \ Q_n = 2|g_1| (1+2n)^{-3/2}.$$

It is easy to see that for the case of $\vartheta = -\pi/2$, we obtain the same results for spectrum and eigenfunctions as it must be.

We thus obtain that for $g_1 > 0$, the spectrum of $\hat{H}_{3,\pm\pi/2}$ is simple, continuous, and given by $\operatorname{spec}\hat{H}_{3,\pm\pi/2} = \mathbb{R}_+$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its generalized eigenfunctions consists of functions

$$U_E(x) = \sqrt{\sigma'(E)}u_1(x; E), E \ge 0$$
.

For $g_1 < 0$, the spectrum of $\hat{H}_{3,\pm\pi/2}$ is simple and given by $\operatorname{spec}\hat{H}_{3,\pm\pi/2} = \mathbb{R}_+ \cup \{\mathcal{E}_n, n \in \mathbb{Z}_+\}$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions consists of functions

$$U_E(x) = \sqrt{\sigma'(E)} u_1(x; E), \ E \ge 0 ,$$

$$U_n(x) = 2|g_1| (1 + 2n)^{-3/2} u_1(x; \mathcal{E}_n), \ \mathcal{E}_n < 0 .$$

We note that the spectrum and eigenfunctions for $\hat{H}_{3,\pi/2}$ coincide with those for \hat{H}_{ϵ} with $g_2 \geq 3/4$, if we set $\mu = 0$ in the respective formulas in subsec. 3.1.

We now turn to the case $|\vartheta| < \pi/2$. In this case, $\sigma'(E)$ can be represented as

$$\sigma'(E) = (\pi \cos^2 \vartheta)^{-1} \operatorname{Im} \left[\omega_3(E + i0) \right]^{-1},$$

$$\omega_3(W) = \psi(\alpha) + \ln(\lambda/k_0) - 2\psi(1) - \tan \vartheta.$$

For $E = p^2 \ge 0, p \ge 0, \lambda = 2pe^{-i\pi/2}, \text{ and } g_1 < 0, \text{ we have}$

$$\sigma'(E) = \frac{B(E)}{\pi \cos^2 \vartheta[A^2(E) + B^2(E)]} , \qquad (41)$$

where $\omega_3(E) = A(E) - iB(E)$. The function B(E) can be explicitly calculated:

$$B(E) = \frac{\pi}{2} \left(1 - \tanh \frac{\pi g_1}{2\sqrt{E}} \right) > 0, \ \forall E \ge 0 \ ,$$
 (42)

whence it follows that for all $E \ge 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is purely continuous. For $E = p^2 > 0$, p > 0, $\lambda = 2pe^{-i\pi/2}$, and $g_1 > 0$, the spectral function is given by the same eqs. (41) and (42). But in this case, B(0) = 0 and the limit $\lim_{W\to 0} \omega_3(W)$ must be carefully examined.

At small W, we have

$$\omega_3(W) = (\tan \vartheta_0 - \tan \vartheta) - \left(6g_1^2\right)^{-1}W + O(W^2), \ \tan \vartheta_0 = \ln(g_1/k_0) - 2\psi(1) \ .$$

For $\vartheta \neq \vartheta_0$, the function $\sigma'(E)$ is finite at E = 0. But for $\vartheta = \vartheta_0$ and small E, we have

$$\sigma'(E) = -\frac{6g_1^2}{\pi \cos^2 \theta_0} \operatorname{Im} (E + i0)^{-1} + O(1) = \frac{6g_1^2}{\cos^2 \theta_0} \delta(E) + O(1) ,$$

which means that the spectrum of the Hamiltonian \hat{H}_{3,ϑ_0} contains an eigenvalue E=0.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\omega_3(E)$ is real, therefore, $\sigma'(E)$ can differ from zero only at zero-points $E_n = E_n(\vartheta)$ of $\omega_3(E)$ ($\omega_3(E_n) = 0$), which yields

$$\sigma'(E) = \sum_{n} \left[-k_0 \omega_3'(E_n) \cos^2 \vartheta \right]^{-1} \delta(E - E_n), \ \omega_3'(E_n) < 0 ,$$

$$\partial_{\vartheta} E_n(\vartheta) = \left[\cos^2 \vartheta \omega_3'(E_n) \right]^{-1} < 0 . \tag{43}$$

For $g_1 > 0$, we have

$$\begin{split} & \omega_3(E) = \psi(1/2 + g_1/2\tau) + \ln(2\tau/g_1) + \tan\vartheta_0 - \tan\vartheta \;, \\ & \omega_3(E) = (1/2) \ln|E| - \tan\vartheta + O(1), \quad E \to -\infty \;, \\ & \omega_3(0) = \tan\vartheta_0 - \tan\vartheta \;. \end{split}$$

For $\vartheta < \vartheta_0$, the equation $\omega_3(E) = 0$ has no solution, whereas for $\vartheta \ge \vartheta_0$, it has only one solution $E^{(-)}(\vartheta)$. Because eq. (43) holds for $\partial_{\vartheta} E^{(-)}(\vartheta)$, $E^{(-)}(\vartheta)$ increases from $-\infty$ to 0 when ϑ changes from $\pi/2 - 0$ to ϑ_0 .

For $g_1 < 0$, we have

$$\omega_3(E) = \psi(1/2 - |g_1|/2\tau) + \ln(2\tau/k_0) - 2\psi(1) - \tan \vartheta ,$$

$$\omega_3(E) = (1/2) \ln |E| - \tan \vartheta + O(1), E \to -\infty .$$

It is easy to verify that the equation $\omega_3(E) = 0$ has an infinite number of solutions $E_n, n \in \mathbb{Z}_+$, bounded from below and asymptotically coinciding with (22) as $n \to \infty$, $E_n = -g_1^2/4n^2 + O(n^{-3})$.

We thus obtain that for $g_1 > 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is simple and given by $\operatorname{spec} \hat{H}_{3,\vartheta} = \mathbb{R}_+ \cup \{E^{(-)}(\vartheta)\}$ and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions consists of functions

$$U_E(x) = \sqrt{\sigma'(E)} u_{3,\vartheta}(x; E), E \ge 0,$$

$$U(x) = \left[-k_0 \cos^2 \vartheta \omega_3'(E^{(-)}(\vartheta)) \right]^{-1/2} u_{3,\vartheta}(x; E^{(-)}(\vartheta)),$$

(the eigenvalue $E^{(-)}(\vartheta)$ exists, and therefore $E^{(-)}(\vartheta)$ and the corresponding eigenfunction U(x) enter the inversion formulas only if $\vartheta \geq \vartheta_0$); for $g_1 < 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is simple and given by $\operatorname{spec}\hat{H}_{3,\vartheta} = \mathbb{R}_+ \cup \{E_n\}$ and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions consists of functions

$$U_E(x) = \sqrt{\sigma'(E)} u_{3,\vartheta}(x; E), \ E \ge 0 ,$$

$$U_n(x) = \left[-k_0 \cos^2 \vartheta \omega_3'(E_n) \right]^{-1/2} u_{3,\vartheta}(x; E_n), \ E_n < 0 .$$

It is possible to describe the discrete spectrum for $|\vartheta| < \pi/2$ and $g_1 < 0$ in more details. To this end, we represent the equation $\omega_3(E) = 0$ in the equivalent form

$$f_3(E) = \tan \vartheta$$
, $f_3(E) = \psi(1/2 - |g_1|/2\tau) + \ln(2\tau/k_0) - 2\psi(1)$.

Then we have

$$f(-\infty) = \infty, \ f(\mathcal{E}_n \pm 0) = \pm \infty, \ n \in \mathbb{Z}_+.$$

Because eq. (43) holds, we can see that in each interval $(\mathcal{E}_n, \mathcal{E}_{n+1})$, $n \in \{-1\} \cup \mathbb{Z}_+$, there is one discrete eigenvalue E_n and E_n increases monotonically from $\mathcal{E}_n + 0$ to $\mathcal{E}_{n+1} - 0$ when ϑ changes from $\pi/2 - 0$ to $-\pi/2 + 0$ (we set $\mathcal{E}_{-1} = -\infty$). We note the relations

$$\lim_{\vartheta \to -\pi/2} E_{n-1}(\vartheta) = \lim_{\vartheta \to \pi/2} E_n(\vartheta) = \mathcal{E}_n .$$

3.4 The fourth range $g_2 < -1/4 \ (\mu = i\varkappa, \varkappa > 0)$

The analysis in this section is completely similar to that in Section 3.2 (although the results for the spectrum differ drastically). We therefore briefly outline basic points.

According to Section (2), the deficiency indices of the initial symmetric operator \hat{H} with $g_2 < -1/4$ are $m_{\pm} = 1$, and therefore there exists a one-parameter family of its s.a. extensions.

To evaluate the asymmetry form Δ_{H^+} , we determine the asymptotics of functions ψ_* belonging to $D_{\dot{H}}^*(\mathbb{R}_+)$ at the origin using representation (23) with $\mu = i\varkappa$ of the general solution of eq. (14) with W = 0 and estimating the integral terms by means of the Cauchy-Bunyakovskii inequality, which yields

$$\psi_*(x) = a_1 u_{1as}(x) + a_2 u_{2as}(x) + O(x^{3/2}), \ x \to 0 ,$$

$$\psi'_*(x) = a_1 u'_{1as}(x) + a_2 u'_{2as}(x) + O(x^{1/2}), \ x \to 0 ,$$

$$u_{1as}(x) = (k_0 x)^{1/2 + i \varkappa}, \ u_{2as}(x) = (k_0 x)^{1/2 - i \varkappa} = \overline{u_{1as}(x)} ,$$

$$(44)$$

and we find⁸ $\Delta_{H^+}(\psi_*) = -2i\varkappa(\overline{a_1}a_1 - \overline{a_2}a_2)$. The requirement that Δ_{H^+} vanish results in the relation $a_1 = e^{2i\theta}a_2$, $\theta \in \mathbb{S}(0,\pi)$ defining the domains of possible s.a. Hamiltonians.

The final result is that: for each g_2 in the range $g_2 < -1/4$, there exists a family of s.a. Hamiltonians $\hat{H}_{4,\theta}$ with the domains

$$D_{H_{4,\theta}} = \left\{ \psi : \psi \in D_{\check{H}}^*(\mathbb{R}_+), \ \psi \text{ satisfies (45)} \right\} ,$$

where (45) are the asymptotic s.a. boundary conditions at the origin

$$\psi = C\psi_{4as}(x) + O(x^{3/2}), \ \psi' = C\psi'_{4as}(x) + O(x^{1/2}), \ x \to 0 ,
\psi_{4as}(x) = e^{i\theta}u_{1as}(x) + e^{-i\theta}u_{2as}(x) = \overline{\psi_{4as}(x)} .$$
(45)

To evaluate the Green's function G(x, y; W) for $\hat{H}_{4,\theta}$, we use representation (15) with $a_1 = 0$ for $\psi_*(x)$ belonging to $D_{H_{4,\theta}} \subset D^*_{\check{H}}(\mathbb{R}_+)$, boundary conditions (26) and asymptotics (44) then yield

$$-a_2 = \frac{2i\varkappa(\lambda k_0)^{-i\chi} e^{-i\theta}}{\omega(W)\omega_{4,\theta}(W)} \int_0^\infty \upsilon_1(x;W)\eta(x)dx, \ \omega_{4,\theta}(W) = a(W) + b(W) ,$$
$$a(W) = e^{i\theta} \frac{\Gamma(\beta)(\lambda/k_0)^{-i\varkappa}}{\Gamma(\alpha)}, \ b(W) = e^{-i\theta} \frac{\Gamma(\beta_-)(\lambda/k_0)^{i\varkappa}}{\Gamma(\alpha_-)} .$$

Using the representation

$$v_1(x;W) = -\frac{(\lambda/k_0)^{i\varkappa}k_0^{-1/2+i\varkappa}}{4\varkappa} \left[i\tilde{\omega}_{4,\theta}(W)u_{4,\theta}(x;W) + \omega_{4,\theta}(W)\tilde{u}_{4,\theta}(x;W) \right] ,$$

⁸This structure of Δ_{H^+} confirms that the deficiency indices of \hat{H} are $m_{\pm}=1$.

where

$$\tilde{\omega}_{4,\theta}(W) = a(W) - b(W), \ \tilde{u}_{4,\theta}(x;W) = i[e^{-i\theta}k_0^{1/2 - i\varkappa}u_2(x;W) - e^{i\theta}k_0^{1/2 + i\varkappa}u_1(x;W)],$$
$$u_{4,\theta}(x;W) = e^{i\theta}k_0^{1/2 + i\varkappa}u_1(x;W) + e^{-i\theta}k_0^{1/2 - i\varkappa}u_2(x;W),$$

where $u_{4,\theta}$ and $\tilde{u}_{4,\theta}$ are solutions of eq. (4) real-entire in W, and $u_{4,\theta}$ satisfies boundary conditions (45), we find

$$\begin{split} G(x,y;W) &= \Omega(W) u_{4,\theta}(x;W) u_{4,\theta}(y;W) \\ &- \frac{1}{4\varkappa k_0} \left\{ \begin{array}{l} \tilde{u}_{4,\theta}(x;W) u_{4,\theta}(y;W), \ x>y \\ u_{4,\theta}(x;W) \tilde{u}_{4,\theta}(y;W), \ x$$

the second summand in G(x, y; W) is real for real W = E.

It is easy to verify that the guiding functional given by (17) with $U = u_{4,\theta}$ satisfies the properties 1)-3) cited in subsec. 3.1, whence it follows that the spectra of $\hat{H}_{4,\theta}$ are simple.

The derivative of the spectral function is given by $\sigma'(E) = \pi^{-1} \operatorname{Im} \Omega(E+i0)$. For $E = p^2 \ge 0$, $p \ge 0$, $\lambda = 2pe^{-i\pi/2}$, and $g_1 < 0$, we have

$$\sigma'(E) = \pi^{-1} \operatorname{Im} \Omega(E) = \frac{\left(4\pi \varkappa k_0\right)^{-1} \left(1 - |D(E)|^2\right)}{\left(1 + D(E)\right)\left(1 + \overline{D}(E)\right)} ,$$

$$D(E) = \frac{a(E)}{b(E)} = \frac{e^{-2i\theta} \Gamma(\beta) \Gamma(\alpha_{-}) e^{2i\varkappa \ln(k_0/2p)} e^{-\pi\varkappa}}{\Gamma(\beta_{-}) \Gamma(\alpha)} .$$

$$(46)$$

Because

$$|D(E)|^2 = \frac{1 + e^{-2\pi\varkappa} e^{-\pi g_1/p}}{1 + e^{2\pi\varkappa} e^{-\pi g_1/p}} < 1, \ \forall p \ge 0 \ , \tag{47}$$

 $\operatorname{spec} H_{4,\theta} = \mathbb{R}_+$ and is simple.

For $E = p^2 > 0$, p > 0, $\lambda = 2pe^{-i\pi/2}$, and $g_1 > 0$ expressions (46) and (47) for $\sigma'(E)$ hold true. But in this case, we have |D(0)| = 1 and must carefully examine the limit $\lim_{W\to 0} \Omega(W)$.

It is easy to see that for small W, we have the representation

$$\Omega(W) = -\frac{i}{4\varkappa k_0} \frac{1 + e^{2i(\theta_0 - \theta)}}{[1 - e^{2i(\theta_0 - \theta)}] + iW/A} + O(1), \ A = \frac{3g_1^2}{\varkappa (1 + 4\varkappa^2)} ,$$

$$\theta_0 = \varphi - \pi[\varphi/\pi], \ \varphi = \varkappa \ln(g_1/k_0) - \theta_\Gamma + \pi/2, \ \theta_\Gamma = \frac{1}{2i} \ln \frac{\Gamma(\beta)}{\Gamma(\beta_-)} ,$$

where $[\varphi/\pi]$ is the entire part of φ/π . For $\theta \neq \theta_0$, the function $\sigma'(E)$ is finite at E = 0. But for $\theta = \theta_0$, we find

$$\sigma'(E+0) = -\pi^{-1} (A/2\varkappa k_0) \operatorname{Im} (E+i0)^{-1} + O(1) = (A/2\varkappa k_0) \delta(E) + O(1) ,$$

which means that the spectrum of the Hamiltonian \hat{H}_{4,θ_0} with $g_1 > 0$ contains the eigenvalue E = 0.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function Ω can be represented as $\Omega(E) = \pi \tan \Theta(E)$, $\Theta(E) = \theta + \theta_{\Gamma} - \theta_{\Gamma}(E) + \varkappa \ln(k_0/2\tau)$,

$$\Omega(E) = \kappa \tan \Theta(E), \ \Theta(E) = \theta + \theta_{\Gamma} - \theta_{\Gamma}(E) + \kappa \sin(\kappa_0/2T)$$

where

$$\theta_{\Gamma}(E) = \frac{1}{2i} \left[\ln \Gamma(1/2 + g_1/2\tau + i\varkappa) - \ln \Gamma(1/2 + g_1/2\tau - i\varkappa) \right]$$

$$= \begin{cases} -\pi |g_1|/2\tau + \varkappa \ln(|g_1|/2\tau) + O(1), \ g_1 < 0 \\ \varkappa \ln(g_1/2\tau) + O(\tau), \ g_1 > 0 \end{cases}, E \to 0$$

$$\theta_{\Gamma}(-\infty) = \frac{1}{2i} \ln \frac{\Gamma(1/2 + i\varkappa)}{\Gamma(1/2 - i\varkappa)} + O(1/\tau), E \to -\infty$$

The asymptotic behavior of $\Theta(E)$ at the origin and at minus infinity is given by

$$\Theta(E) = \begin{cases} \pi |g_1|/2\tau + O(1), \ g_1 < 0 \\ \theta + \theta_{\Gamma} + \varkappa \ln(k_0/g_1) + O(\tau), \ g_1 > 0 \end{cases}, E \to 0 \\ \theta + \theta_{\Gamma} - \theta_{\Gamma}(-\infty) + \varkappa \ln(k_0/2\tau) + O(1/\tau), E \to -\infty \end{cases}$$

Because $\Omega(E)$ is a real function for E < 0, $\sigma'(E)$ can differ from zero only at the points $E_n = E_n(\theta)$ where $\Theta(E_n) = \pi/2 + \pi n$, $n \in \mathbb{Z}$, which yields

$$\sigma'(E) = \sum_{n} Q_n^2 \delta(E - E_n), \ Q_n = \left[4\varkappa k_0 \Theta'(E_n)\right]^{-1/2}, \ \Theta'(E_n) > 0.$$

We can obtain an additional information about the discrete spectrum of $\hat{H}_{4,\theta}$. Representing the equation $\Theta(E_n) = \pi/2 + \pi n$, $n \in \mathbb{Z}$, in the equivalent form

$$f_4(E_n) = \pi/2 + \pi(n - \theta/\pi), \ f_4(E) = \theta_{\Gamma} - \theta_{\Gamma}(E) + \varkappa \ln(k_0/2\tau),$$

$$\partial_{\theta} E_n(\theta) = -\left[f_4'(E_n(\theta))\right]^{-1} = -\left[\Theta'(E_n(\theta))\right]^{-1} < 0,$$

we can see that the following assertions hold.

- a) The eigenvalue $E_n(\theta)$ with fixed n decreases monotonically from $E_n(0)$ to $E_n(\pi) 0$ when θ changes from 0 to $\pi 0$. In particular, we have $E_{n-1}(\theta) < E_n(\theta), \forall n$.
- b) For any g_1 , the spectrum is unbounded from below: $E_n \to -\infty$ as $n \to -\infty$.
- c) For any θ , the negative part of the spectrum is of the form $E_n = -k_0^2 m^2 e^{2\pi |n|/\varkappa} (1 + O(1/n))$ as $n \to -\infty$, where $m = m(g_1, g_2, \theta)$ is a scale factor, and asymptotically (as $n \to -\infty$) coincides with the negative part of the spectrum in the Calogero model with coupling constant g_2 under an appropriate identification of scale factors.
- d) For $g_1 < 0$, the discrete part of the spectrum has an accumulation point E = 0. More specifically, the spectrum is of the form $E_n = -g_1^2/4n^2 + O(1/n^3)$ as $n \to \infty$ (as in all the previous ranges of the parameter g_2) and asymptotically coincides with the spectrum for $g_2 = 0$, see below.

e) For $g_1 > 0$, the discrete spectrum has no finite accumulation points. In particular, possible values of n are restricted from above, $n \leq n_{\text{max}}$, where

$$n_{\rm max} = \left\{ \begin{array}{l} f_4(0)/\pi - 1/2 \ {\rm if} \ f_4(0)/\pi - 1/2 \ {\rm is \ integer} \\ [f_4(0)/\pi + 1/2] \ {\rm if} \ f_4(0)/\pi - 1/2 > [f_4(0)/\pi - 1/2] \end{array} \right. ,$$

and the level E=0 is present in the spectrum for $\theta=\theta_0$ only.

The final result is as follows: the spectrum of $\hat{H}_{4,\theta}$ is simple and given by $\operatorname{spec}\hat{H}_{4,\theta} = \mathbb{R}_+ \cup \{E_n \leq 0\}, \ -\infty < n < n_{\max}, \text{ where } n_{\max} < \infty \text{ for } g_1 > 0$ and $n_{\max} = \infty$ for $g_1 < 0$, and the set of the corresponding (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}u_{4,\theta}(x;E), E \ge 0; U_n(x) = Q_n u_{4,\theta}(x;E_n), E_n \le 0,$$

form a complete orthonormalized system in $L^{2}(\mathbb{R}_{+})$.

3.5 The fifth range $g_2 = 0$ ($\mu = 1/2$)

The analysis in this section is similar to that in subsec. 3.2. A peculiarity is that the function u_2 is not defined for $\mu = 1/2$, and we therefore use the following solutions of eq. (4):

$$u_1(x;W) = xe^{-z/2}\Phi(\alpha_{1/2},2;z), \ u_5(x;W) = \tilde{u}_5(x;W) - g_1 \ln k_0 u_1(x;W) ,$$

$$v_1(x;W) = xe^{-z/2}\Psi(\alpha_{1/2},2;z) = \Gamma^{-1}(\alpha_{1/2}) \left[\omega_{1/2}(W) u_1(x;W) + u_5(x;W) \right] ,$$

where

$$\begin{split} &\alpha_{1/2} = 1 + g_1/\lambda, \\ &\tilde{u}_5(x;W) = \mathrm{e}^{-z/2} x^{1/2} \left[x^{-\mu} \Phi(\alpha_-,\beta_-;z) + g_1 \Gamma(\beta_-) x^{\mu} \Phi(\alpha_+,\beta_+;z) \right]_{\mu \to 1/2} \;, \\ &\omega_{1/2}(W) = g_1 \mathbf{C} + g_1 \left[\psi(\alpha_{1/2}) + \ln(\lambda/k_0) \right] - g_1 - \lambda/2 \;, \end{split}$$

C is the Euler constant. The asymptotics of these functions at the origin and at infinity are respectively as follows.

As
$$x \to 0$$
, $z = \lambda x \to 0$, we have

$$u_{1}(x;W) = k_{0}^{-1}u_{1as}(x) + O(x^{2}), \ u_{5}(x;W) = u_{5as}(x) + O(x^{2}\ln x) ,$$

$$v_{1}(x;W) = \Gamma^{-1}(\alpha_{1/2}) \left[k_{0}^{-1}\omega_{1/2}(W)u_{1as}(x) + u_{5as}(x) \right] + O(x^{2}\ln x) ,$$

$$u_{1as}(x) = k_{0}x, \ u_{5as}(x) = 1 + g_{1}x\ln(k_{0}x) + \mathbf{C}g_{1}x .$$
(48)

As $x \to \infty$, Im W > 0, we have

$$\begin{split} u_1(x;W) &= \Gamma^{-1}(\alpha_{1/2}) \lambda^{-1+g_1/\lambda} x^{+g_1/\lambda} \mathrm{e}^{z/2} (1 + O(x^{-1})) \to \infty , \\ v_1(x;W) &= \lambda^{-g_1/\lambda} x^{-g_1/\lambda} \mathrm{e}^{-z/2} (1 + O(x^{-1})) \to 0 . \end{split}$$

The functions $u_1(x; W)$ and $u_5(x; W)$ are real-entire in W. These functions form a fundamental system of solutions of eq. (4), the same holds for the functions u_1, v_1 for Im $W \neq 0$, see subsec. 3.2,

Wr
$$(u_1, u_5) = -1$$
, Wr $(u_1, v_1) = -1/\Gamma(\alpha_{1/2}) = -\omega(W)$.

As we know from subsec. 3.2, for $g_2 < -1/4$, the deficiency indices of the initial symmetric operator \hat{H} are $m_{\pm} = 1$, and therefore there exists a one-parameter family of its s.a. extensions.

For evaluating the asymmetry form Δ_{H^+} , we determine the asymptotics of functions ψ_* , belonging to $D_{\tilde{H}}^*(\mathbb{R}_+)$, at the origin using representation (23) of the general solution of eq. (14) with W=0, where the natural substitutions $a_2u_2 \to a_2u_5$ and $u_2/2\mu \to u_5$ must be made, and estimating the integral terms by means of the Cauchy-Bunyakovskii inequality, which yields

$$\psi_*(x) = a_1 u_{1as}(x) + a_2 u_{5as}(x) + O(x^{3/2}) ,$$

$$\psi_*'(x) = a_1 u_{1as}'(x) + a_2 u_{5as}'(x) + O(x^{1/2}) ,$$
 (49)

and we find 9 $\Delta_{H^{+}}(\psi_{*}) = -k_{0}(\overline{a_{1}}a_{2} - \overline{a_{2}}a_{1})$. The requirement that $\Delta_{H^{+}}$ vanish results in the relation $a_{1}\cos\epsilon = a_{2}\sin\epsilon$, $\epsilon \in \mathbb{S}(-\pi/2, \pi/2)$.

The final result is that for $g_2=0$, there exists a family of s.a. Hamiltonians $\hat{H}_{5,\epsilon}$ with the domains

$$D_{H_{5,\epsilon}} = \left\{ \psi : \psi \in D_{\check{H}}^*(\mathbb{R}_+), \ \psi \text{ satisfies (50)} \right\} ,$$

where (50) are the asymptotic s.a. boundary conditions at the origin

$$\psi = C\psi_{5,\epsilon_{as}}(x) + O(x^{3/2}), \ \psi' = C\psi'_{5,\epsilon_{as}}(x) + O(x^{1/2}), \ x \to 0 ,$$

$$\psi_{5,\epsilon_{as}}(x) = u_{1as}(k_0 x) \sin \epsilon + u_{5as}(x) \cos \epsilon .$$
 (50)

To find the Green's function G(x, y; W) for $\hat{H}_{5,\epsilon}$, we use representation (15) with $a_1 = 0$ for $\psi_*(x)$ belonging to $D_{H_{4,\theta}} \subset D^*_{\check{H}}(\mathbb{R}_+)$, boundary conditions (50) and asymptotics (48) then yield

$$a_2 = -\frac{\Gamma^2(\alpha_{1/2})\cos\epsilon}{\omega_{1/2}(W)\cos\epsilon - k_0\sin\epsilon} \int_0^\infty \upsilon_1(x;W)\eta(x)dx .$$

Using the representation

$$\begin{split} k_0\Gamma(\alpha_{1/2})\upsilon_1(x;W) &= (\omega_{1/2}(W)\cos\epsilon - k_0\sin\epsilon)\tilde{u}_{5,\epsilon}(x;W) \\ &+ (\omega_{1/2}(W)\sin\epsilon + k_0\cos\epsilon)u_{5,\epsilon}(x;W) \;, \\ u_{5,\epsilon}(x;W) &= k_0u_1(x;W)\sin\epsilon + u_5(x;W)\cos\epsilon \;, \\ \tilde{u}_{5,\epsilon}(x;W) &= k_0u_1(x;W)\cos\epsilon - u_5(x;W)\sin\epsilon \;, \end{split}$$

⁹This structure of Δ_{H^+} confirms that the deficiency indices of \hat{H} are $m_{\pm}=1$.

where $u_{5,\epsilon}(x;W)$ and $\tilde{u}_{5,\epsilon}(x;W)$ are solutions of eq. (4) real-entire in W and $u_{5,\epsilon}(x;W)$ satisfies boundary conditions (50), we find

$$\begin{split} G(x,y;W) &= \frac{1}{k_0} \left[\Omega(W) u_{5,\epsilon}(x;W) u_{5,\epsilon}(y;W) - \left\{ \begin{array}{l} \tilde{u}_{5,\epsilon}(x;W) u_{5,\epsilon}(y;W), \ x > y \\ u_{5,\epsilon}(x;W) \tilde{u}_{5,\epsilon}(y;W), \ x < y \end{array} \right], \\ \Omega(W) &= \left[k_0 \sin \epsilon - \omega_{1/2}(W) \cos \epsilon \right]^{-1} \left[\omega_{1/2}(W) \sin \epsilon + k_0 \cos \epsilon \right] \ , \end{split}$$

the second summand in G(x, y; W) is real for real W = E.

It is easy to verify that the guiding functional given by (17) with $U = u_{5,\epsilon}$ satisfies the properties 1)-3) cited in subsec. 3.1, whence it follows that the spectra of $\hat{H}_{5,\epsilon}$ are simple.

The derivative of the spectral function is given by $\sigma'(E) = (\pi k_0)^{-1} \operatorname{Im} \Omega(E + i0)$.

We first consider the case of $\epsilon=\pi/2$ where we have $u_{5,\pi/2}(x;W)=k_0u_1(x;W)$ and

$$\sigma'(E) = (\pi k_0^2)^{-1} \operatorname{Im} \tilde{\Omega}(E + i0) ,$$

$$\tilde{\Omega}(W) = g_1 \psi(\alpha_{1/2}) + g_1 \ln(\lambda/k_0) - \lambda/2 .$$

For $E = p^2 > 0$, p > 0, $\lambda = 2pe^{-i\pi/2}$, we have

$$\sigma'(E) = \frac{|g_1| e^{-\pi g_1/2p}}{2k_0^2 \sinh(\pi |g_1|/2p)} \ge 0.$$

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, and $g_1 > 0$, $\alpha_{1/2} = 1 + g_1/2\tau$, the function $\tilde{\Omega}(E)$ is finite and real, whence it follows that there are no negative spectrum points.

For
$$E = -\tau^2 < 0$$
, $\tau > 0$, $\lambda = 2\tau$, and $g_1 < 0$, $\alpha_{1/2} = 1 - |g_1|/2\tau$, we have
$$\sigma'(E) = -\left(\pi k_0^2\right)^{-1} |g_1| \operatorname{Im} \psi(\alpha)|_{W=E+i0} = \sum_{n \in \mathbb{Z}_+} Q_n^2 \delta(E - \mathcal{E}_n) ,$$

$$\mathcal{E}_n = -\frac{g_1^2}{(2+2n)^2}, \ Q_n = \frac{2}{k_0} \left(\frac{|g_1|}{2+2n}\right)^{3/2} .$$

It is easy to see that for the case of $\epsilon = -\pi/2$, we obtain the same results for spectrum and eigenfunctions as it must be.

We thus obtain that for $g_1 > 0$, the spectrum of $H_{5,\pi/2}$ is simple, continuous, and given by $\operatorname{spec} \hat{H}_{5,\pm\pi/2} = \mathbb{R}_+$ and the set of generalized eigenfunctions $U_E(x) = \sqrt{\sigma'(E)} u_{5,\pi/2}(x;E), E \geq 0$, form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

For $g_1 < 0$, the spectrum of $H_{5,\pm\pi/2}$ is simple and given by $\operatorname{spec} H_{5,\pm\pi/2} = \mathbb{R}_+ \cup \{\mathcal{E}_n, \ n \in \mathbb{Z}_+\}$ and the set of (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} u_{5,\pi/2}(x; E), E \ge 0,$$

$$U_n(x) = \frac{2}{k_0} \left(\frac{|g_1|}{2+2n}\right)^{3/2} u_{5,\pi/2}(x; \mathcal{E}_n),$$

form a complete orthonormalized system in $L^{2}(\mathbb{R}_{+})$.

We now turn to the case $|\epsilon| < \pi/2$ where we have

$$\sigma'(E) = (\pi \cos^2 \epsilon)^{-1} \operatorname{Im} [\omega_5(E+i0)]^{-1}, \quad \omega_5(W) = k_0 \tan \epsilon - \omega_{1/2}(W).$$

For $g_1 < 0$, $E = p^2 \ge 0$, $p \ge 0$, $\lambda = 2pe^{-i\pi/2}$, we obtain that

$$\sigma'(E) = (\pi \cos^2 \epsilon)^{-1} \operatorname{Im} \omega_5^{-1}(E) = \frac{B(E)}{\pi \cos^2 \epsilon [A^2(E) + B^2(E)]} , \qquad (51)$$

where $\omega_5(E) = A(E) - iB(E)$. The function B(E) is explicitly given by

$$B(E) = \frac{\pi}{2} \frac{|g_1| e^{-\pi g_1/2p}}{\sinh(\pi |g_1|/2p)} > 0, \ \forall p \ge 0.$$
 (52)

It follows that for $g_1 < 0$, $E \ge 0$, the spectrum of $\hat{H}_{5,\epsilon}$ is purely continuous. For $g_1 > 0$, $E = p^2 > 0$, p > 0, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, the derivative of the spectral function is also given by eqs. (51) and (52). But in this case, we have B(0) = 0 and the limit $\lim_{W\to 0} \omega_5(W)$ has to be carefully examined. For small W, we have

$$\omega_5(W) = (\tan \epsilon - \tan \epsilon_0)k_0 - \frac{1}{3g_1}W + O(W^2),$$

 $\tan \epsilon_0 = (g_1/k_0)[\ln(g_1/k_0) + \mathbf{C} - 1].$

For $\epsilon \neq \epsilon_0$, the function $\sigma'(E)$ has a finite limit as $E \to 0$. But for $\epsilon = \epsilon_0$ and small E, we have

$$\sigma'(E) = -\frac{3g_1}{\pi \cos^2 \epsilon_0} \operatorname{Im} (E + i0)^{-1} + O(1) = \frac{3g_1}{\cos^2 \epsilon_0} \delta(E) + O(1) ,$$

which means that the spectrum of the Hamiltonian \hat{H}_{5,ϵ_0} has an eigenvalue E=0.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\omega_5(E)$ is real. Therefore, $\sigma'(E)$ can differ from zero only at zero points $E_n = E_n(\epsilon)$ of $\omega_5(E)$, and $\sigma'(E)$ is represented as

$$\sigma'(E) = \sum_{n} \left[-\omega_5'(E_n) \right]^{-1} \delta(E - E_n), \ \omega_5(E_n) = 0, \ \omega_5'(E_n) < 0.$$

For $q_1 > 0$, we have

$$\omega_5(E) = -g_1 \psi(1 + g_1/2\tau) - g_1 \ln(2\tau/g_1) + \tau + k_0 (\tan \epsilon - \tan \epsilon_0) ,$$

$$\omega_5(E) = \sqrt{|E|} - (g_1/2) \ln|E| + O(1), \quad E \to -\infty; \quad \omega_5(0) = k_0 (\tan \epsilon - \tan \epsilon_0) .$$

For $\epsilon > \epsilon_0$, the equation $\omega_5(E) = 0$ has no solution, while for $\epsilon \in (-\pi/2, \epsilon_0]$ it has a unique solution $E^{(-)}(\epsilon)$. It is easy to see that

$$\partial_{\epsilon} E^{(-)}(\epsilon) = -k_0 \left[\omega_5'\left(E_{\epsilon}^{(-)}\right)\cos^2\epsilon\right]^{-1} > 0$$

so that $E^{(-)}(\epsilon)$ increases monotonically from $-\infty$ to 0 when ϵ changes from $-\pi/2 + 0$ to ϵ_0 .

For $g_1 < 0$, we have

$$\omega_5(E) = |g_1|\psi(1/2 - |g_1|/2\tau) + |g_1|\ln(2\tau/k_0) + \tau - \tilde{\epsilon},$$

 $\tilde{\epsilon} = g_1\mathbf{C} - g_1 - k_0 \tan \epsilon.$

Representing the equation $\omega_5(E_n) = 0$ in the equivalent form

$$f_5(E_n) = \tilde{\epsilon}, \ f_5(E) = |g_1|\psi(1/2 - |g_1|/2\tau) + |g_1|\ln(2\tau/k_0) + \tau$$

we can see that:

a) $f_5(E) \stackrel{E \to -\infty}{\longrightarrow} \infty, \quad f_5(\mathcal{E}_n \pm 0) = \pm \infty ,$

such that in each region of energy $(\mathcal{E}_n, \mathcal{E}_{n+1})$, $n \in (-1) \cup \mathbb{Z}_+$, the equation $\omega_5(E_n) = 0$ has one solution $E_n(\epsilon)$ for any fixed ϵ , $|\epsilon| < \pi/2$, and $E_n(\epsilon)$ increases monotonically from $\mathcal{E}_n + 0$ to $\mathcal{E}_{n+1} - 0$ as ϵ changes from $-\pi/2 + 0$ to $\pi/2 - 0$ (here, by the definition, $\mathcal{E}_{-1} = -\infty$).

- b) For any fixed ϵ , $E_n(\epsilon) = -g_1^2/4n^2 + O(n^{-3})$ as $n \to \infty$, asymptotically coinciding with (22).
- c) The point E = 0 is an accumulation point of discrete spectrum for $g_1 < 0$.

Note the relation

$$\lim_{\epsilon \to \pi/2} E_{n-1}(\epsilon) = \lim_{\epsilon \to -\pi/2} E_n(\epsilon) = \mathcal{E}_n, \ n \in \mathbb{Z}_+ \ .$$

The above results can be briefly summarized as follows.

For $g_1 < 0$, the spectrum of $\hat{H}_{5,\epsilon}$ is simple and given by $\operatorname{spec}\hat{H}_{5,\epsilon} = \mathbb{R}_+ \cup \{E_n < 0, n \in (-1) \cup \mathbb{Z}_+\}$. The (generalized) eigenfunctions

$$U_{E}(x) = \sqrt{\sigma'(E)} u_{5,\epsilon}(x; E), \ E \ge 0 ,$$

$$U_{n}(x) = \left[-\omega'_{5,\epsilon}(E_{n}) \right]^{-1/2} u_{5,\epsilon}(x; E_{n}), \ E_{n} < 0, \ n \in (-1) \cup \mathbb{Z}_{+} ,$$

form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

For $g_1 > 0$, the spectrum of $\hat{H}_{5,\epsilon}$ is simple and given by $\operatorname{spec} \hat{H}_{5,\epsilon} = \mathbb{R}_+ \cup \{E^{(-)}(\epsilon) \leq 0\}$. For $\epsilon \in (-\pi/2, \epsilon_0]$ the (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} u_{5,\epsilon}(x; E), \ E \ge 0, \ U(x) = \left[-\omega_5'(E^{(-)}) \right]^{-1/2} u_{5,\epsilon}\left(x; E^{(-)}\right)$$

form a complete orthonormalized system in $L^{2}(\mathbb{R}_{+})$. For $\epsilon > \epsilon_{0}$, the spectrum has no negative eigenvalues.

We note that the above results (for spectrum and eigenfunctions) can be extracted from the results in subsec. 3.2 for the case $g_2 \neq 0$ ($\mu \neq 1/2$).

4 Some concluding remarks

We would like to finish our consideration with a remark about the Kratzer potential [1] mentioned in the Introduction. This potential corresponds to a particular case of parameters $g_2 > 0$ and $g_1 < 0$. It is drown by the thick line in the graph of Figure 1. As was already said, the Kratzer potential is extensively used to describe the molecular structure and interactions [16]. In such cases, the Kratzer potential appears in the radial part of the Schrödinger equation (2) and has the form:

 $V(x) = -2D_e \left(\frac{a}{x} - \frac{1}{2}\frac{a^2}{x^2}\right) , {53}$

where D_e is the dissociation energy and a is the equilibrium inter-nuclear separation. As x goes to zero, V(x) goes to infinity, describing the internuclear repulsion and, as x goes to infinity, V(x) goes to zero, describing the decompositions of molecules. Putting the potential (53) in the radial equation (2) and comparing with the Schrödinger equation (4), we have the following identification:

$$g_1 = -\frac{4m}{\hbar^2} D_e a$$
, $g_2 = \frac{2m}{\hbar^2} D_e a^2 + l(l+1)$.

We can now calculate the value of g_2 for real diatomic molecules. Using data from [20], even for l=0, we have $g_2=4.53\times 10^4$ for CO. The parameter g_2 is of the same order for molecules of NO, O_2 , I_2 , and I_3 . Thus, we can see that for the realistic Kratzer potentials, the corresponding radial equations have always $g_2>3/4$. Thus, the corresponding radial problem belongs to the first range described in subsec. 3.1. In this case, there exist only one s.a. radial Hamiltonian defined on the natural domain (5), functions from this domain have asymptotics (16).

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References

- A. Kratzer, Die ultraroten Rotationsspektren der Halogenwasserstoffe, Z. Phys 3, 289 (1920)
- [2] E.C. Baughan, Comments on the thermochemistry of the elements of Groups IVB and IV, Quart. Rev. 7, 103 (1953)
- [3] E. Fues, Ueber die Bestimmung der mittleren Wärme der Luft, Ann. Physik 80, 376 (1926)
- [4] C.J. Ballhausen and M. Gajhede, The tunnel effect and scattering by a negative Kratzer potential, Chemical Physics Letters 165, Issue 5, 449 (1990)

- [5] O. Bayrak I. Boztosun and H. Ciftci, Exact Analytical Solutions to the Kratzer Potential by the Asymptotic Iteration Method, Int J Quantum Chem 107, 540 (2007)
- [6] G.H. Shortley, The inverse-cube force in quantum mechanics, Phys. Rev. 38, 120 (1931)
- [7] S.L. Scarf, Discrete States for Singular Potential Problems, Phys.Rev. 109, 2170 (1958)
- [8] L.D. Landau and E.M. Lifshitz, Quantum Mechanics (Pergamon Press 1977).
- [9] M.A. Eliashevich, *Atomic and Molecular Spectroscopy* (State Physical and Mathematical Publishing, Moscow, 1962)
- [10] S. Flügge, Practical Quantum Mechanics; Vol I (Springer: Berlin, 1994)
- [11] H.S.W. Massey, *Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949)
- [12] B.L. Voronov, D.M. Gitman, and I.V. Tyutin, Constructing Quantum Observables and Self-Adjoint Extensions of Symmetric Operators. I, Russian Physics Journal 50/1, 1 (2007); Constructing Quantum Observables and Self-Adjoint Extensions of Symmetric Operators. II. Differential Operators, Russian Physics Journal 50/9, 853 (2007); Constructing quantum observables and self-adjoint extensions of symmetric operators. III. Self-adjoint boundary conditions, Russian Physics Journ. 51/2, 115 (2008)
- [13] J. von Neumann, Zur Algebra der Funktionaloperationen und Theorie der normalen Operatoren, Math. Ann. 102, 370 (1929)
- [14] M.T. Krein, One general method of decompositions of positively defined kernals in elementar products, DAN USSR 53, 3 (1946); Hermitian operators with guiding functionals, Zbirnik Prazc' Institutu Matematiki, AN USR No.10, 83 (1948)
- [15] M.A. Naimark, Linear Differential Operators (Nauka, Moscow 1969); N.I. Akhiezer and I.M. Glazman, Theory of Linear Operators in Hilbert Space (Pitman, Boston 1981)
- [16] R.J. Le Roy, R.B. Bernstain, Dissociation Energy and Long-Range Potential of Diatomic Molecules from Vibrational Spacings of Higher Levels, J. Chem. Phys. 52, 3869 (1970)
- [17] J. Vigo-Aguiar, T. E. Simos, Review of multistep methods for the numerical solution of the radial Schrödinger equation, Int J Quantum Chem 103, 278 (2005)
- [18] H. Bateman and A. Erdelyi, *Higher Transcedental Functions* (Mc GRAW-HILL, New York, 1953)

- [19] Gradshtein I.S., Ryzhik N.M. Tables of Integrals, Sums, Series and Products. Nauka, Moscow, 1971.
- [20] M. Karplus, R.N. Porter, Atoms and Molecules (WA Benjamin: Menlo Park, CA, 1970)
- [21] M. Reed and B. Simon, Methods of Modern Mathematical Physics vol 2 Harmonic Analysis. Self-adjointness (New York: Academic,1972)
- [22] V.G. Bagrov and D.M. Gitman, Exact Solutions of Relativistic Wave Equations, (Kluwer, Dordrecht, Boston, London 1990)
- [23] J. von Neumann, Mathematical Foundations of Quantum Mechanics (Princeton University Press, Princeton 1955)
- [24] B.L. Voronov, D.M. Gitman and I.V. Tyutin, The Dirac Hamiltonian with a superstrong Coulomb field, Theor. Math. Phys. 150 34 (2007); Self-adjoint extensions and spectral analysis in Calogero problem, J. Phys. A 43, 145205 (2010)
- [25] D.M. Gitman, I.V. Tyutin, A.G. Smirnov, and B.L. Voronov, Self-adjoint Schrödinger and Dirac operators with Aharonov-Bohm and magneticsolenoid fields, arXiv:0911.0946 [quant-ph] (2009)