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 non-relativistic 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 self-adjoint extensions by (asymptotic) self-adjoint boundary conditions. Solving spectral problems, we follow Krein’s method of guiding functionals. This work is a continuation of our previous works devoted to the Coulomb, Calogero and Aharonov–Bohm potentials.

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1. Introduction

In this paper, we present a mathematically rigorous quantum-mechanical (QM) treatment of a one-dimensional (1D) non-relativistic motion on a semiaxis of a spinless particle of mass $m$ in the potential field

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

At 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, [1, 2] and the books [3–5]. In particular, this potential enters the stationary radial Schrödinger equation

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

where $n$ and $l$ are radial and angular quantum numbers, after separating spherical variables in 3D spherically symmetric QM problems; see, for example, [4]. 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 [6]. The Kratzer potential is conventionally used to describe the molecular energy spectrum, interactions between different molecules [7] and interactions between nonbonded atoms [8]. 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 [9] and decays, in particular, molecule ionization and fluorescence [10]. In addition, valence electrons in a hydrogen-like atom are described in terms of such a potential [11]. When modeling some physical systems, a constant is usually added to the angular momentum term, $l(l+1) \to \beta + l(l+1)$, in order to take some effective potential energy into account. For example, in the model of a...
molecule interaction, $\beta$ can represent the dissociation energy of a diatomic molecule [7]; in the scattering problem, this parameter represents attractive ($\beta < 0$) or repulsive ($\beta > 0$) interactions between charged particles [9].

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

Even though a number of works are 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 paper) is to construct all self-adjoint (referred to as s.a.) 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 to specify s.a. differential operators by (asymptotic) s.a. boundary conditions (the so-called alternative method; see [12]). When solving spectral problems, we follow Krein’s method of guiding functionals; see [13] and the books [14]. This work is a continuation of our previous works [15, 16] devoted to the Coulomb, Calogero and Aharonov–Bohm potentials; using the given references, the reader can become acquainted with the necessary basic notions and constructions, such as the guiding functional and Green’s function.

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

$$\hat{H} = -d_1^2 + g_1 x^{-1} + g_2 x^{-2},$$  

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

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

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

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

$$D^+_H(\mathbb{R}_+) = \{\psi_\alpha(x); \psi_\alpha' \text{ are a.c. in } \mathbb{R}_+; \psi_\alpha, \hat{H}^+\psi_\alpha \in L^2(\mathbb{R}_+)\},$$

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

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

where $\hat{H}$ acts as $\hat{H}^+$. It is evident that $D(\mathbb{R}_+) \subset D^+_H(\mathbb{R}_+)$ and $\hat{H} \subset \hat{H}^+$. The operator $\hat{H}^+$ is generally not s.a.. Its quadratic asymmetry form is denoted by $D_{\Delta H}$. All possible s.a. Hamiltonians associated with $\hat{H}$ are defined as s.a. restrictions of $\hat{H}^+$ (which are simultaneously s.a. extensions of the symmetric $\hat{H}$) to some subspaces (domains) belonging to $D^+_H(\mathbb{R}_+)$ and specified by some additional (asymptotic) boundary conditions on functions belonging to $D^+_H(\mathbb{R}_+)$ under which the asymmetry form $D_{\Delta H}$ becomes trivial (vanishes). These domains are maximum subspaces in $D^+_H(\mathbb{R}_+)$ where the operator $\hat{H}^+$ is symmetric$^4$ (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 [15]; we therefore keep $g_1 \neq 0$ in what follows.

To organize this paper, we present and discuss some exact solutions of equation (4) and their asymptotics. The following five sections, we construct all s.a. extensions of $\hat{H}$ and perform the corresponding spectral analysis of the Hamiltonians for different ranges of the parameter $g_2$. In sections (3.1)–(3.4), we consider the case of $g_2 \neq 0$. The special case of $g_2 = 0$ is considered in section 3.5. In section 4, we make some remarks and highlight 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 $\psi(x)$,

$$z = \lambda x, \quad \lambda = 2 \sqrt{-W} = 2 \sqrt{|W| e^{i(\varphi - \pi)/2}},$$

$$\psi(x) = x^{1/2 - \mu} e^{-\varphi/2} \phi_{\pm}(z),$$

$$\mu = \begin{cases} \sqrt{g_2 + 1/4}, & g_2 \geq -1/4, \\ \text{i} \kappa, & \kappa = \sqrt{|g_2| - 1/4}, \quad g_2 < -1/4, \end{cases}$$

$^3$ a.c. means absolutely continuous.

$^4$ Although the notions ‘s.a. extension of $\hat{H}$’ and ‘s.a. restriction of $\hat{H}^+$’ are equivalent, it is more customary to speak of s.a. extensions; we use one or the other of the equivalent notions where appropriate.

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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).
we reduce equation (4) to the confluent hypergeometric equations for $\phi_±(z)$,

$$z d^2 \phi_±(z) + (\beta_± - z) d \phi_±(z) - \alpha_± \phi_±(z) = 0,$$

$$\alpha_± = 1/2 \pm \mu + g_1/\lambda, \quad \beta_± = 1 \pm 2\mu,$$  

(8)

whose solutions are the known confluent hypergeometric functions $\phi(\alpha_±, \beta_±; z)$ and $\Psi(\alpha_±, \beta_±; z)$; see [17, 18].

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

$$u_1(x; W) = x^{1/2+\mu} e^{-z/2} \Phi(\alpha_+, \beta_+; z) = u_1(x; W)|_{\lambda \to \lambda - 1},$$

$$u_2(x; W) = x^{1/2-\mu} e^{-z/2} \Phi(\alpha_-, \beta_-; z) = u_2(x; W)|_{\lambda \to \lambda - 1} = u_1(x; W)|_{\mu \to -\mu},$$

(9)

$$v_1(x; W) = \lambda x^{1/2+\mu} e^{-z/2} \Psi(\alpha_+, \beta_+; z)$$

$$= \lambda^{1/2} \Gamma(2\mu) \Gamma(\alpha_-) u_1 + \Gamma(2\mu) u_2.$$  

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 $\mu$, we replace $u_2$ by other solutions of equation (4); they are considered in the subsequent sections.

The coefficients of the Taylor expansion of the 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 $\lambda$. Because these are even in $\lambda$, the coefficients are polynomials in $W$, whereas 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 $g_2 \geq -1/4 (\mu > 0)$, then $u_1(x; W)$ and $u_2(x; W)$ are real-entire functions of $W$. If $g_2 < -1/4 (\mu = i\pi)$, then $u_2(x; W)$ is $u_1(x; W)$.

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

$$\text{Wr}(u_1, u_2) = -2\mu,$$

$$\text{Wr}(u_1, v_1) = -\Gamma(\beta_+) / \Gamma(\alpha_+) = -\omega(W).$$

(10)

The well-known asymptotics of the special functions $\Phi$ and $\Psi$, see e.g. [17], entering solutions (9) allows us to simply estimate 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

$$u_1(x; W) = \kappa_0^{1/2-\mu} u_{1w}(x) + O(x^{3/2+\mu}),$$

$$u_2(x; W) = \kappa_0^{1/2-\mu} u_{2w}(x)$$

$$+ \begin{cases} O(x^{5/2-\mu}), & -1/4 < g_2 < 3/4, \quad g_2 \neq 0, \\ 0 < \mu < 1, \mu \neq 1/2, \\ O(x^{3/2}), \quad g_2 < -1/4 (\mu = i\pi), \end{cases}$$

(11)

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

$$v_1(x; W) =$$

$$\frac{\Gamma(2\mu)}{\Gamma(\alpha_+)} x^{1/2-\mu} O(x),$$

$$g_2 \geq 3/4 \quad (\mu > 1)$$

$$\frac{\lambda^{2i\pi} \Gamma(-2i\mu/\mu)}{\Gamma(\alpha_+)} \kappa_0^{-1/2-\mu} u_{1w}(x)$$

$$+ O(x^{3/2}), \quad -1/4 < g_2 < 3/4,$$

$$g_2 \neq 0 \quad (0 < \mu < 1, \mu \neq 1/2),$$

$$\frac{\lambda^{2i\pi} \Gamma(-2i\mu/\mu)}{\Gamma(\alpha_+)} \kappa_0^{-1/2-i\mu} u_{2w}(x)$$

$$+ O(x^{3/2}), \quad g_2 < -1/4 (\mu = i\pi),$$

where $O(x) = 1 + O(x)$,

$$u_{1w}(x) = \frac{\kappa_0(x)^{1/2-\mu}}{\Gamma(\alpha_+)}$$

$$\begin{cases} \frac{g_1/k_0}{2\mu - 1} (\kappa_0 x)^{3/2-\mu}, & -1/4 < g_2 < 3/4, \quad g_2 \neq 0 \\ (0 < \mu < 1, \mu \neq 1/2), \\ \kappa_0(x)^{1/2-i\mu}, \quad g_2 < -1/4 \quad (\mu = i\pi), \end{cases}$$

(13a)

and $k_0$ is an arbitrary, but fixed, parameter of dimension of inverse length.

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

$$u_1(x; W) = \frac{\Gamma(\beta_+)}{\Gamma(\alpha_+)} x^{\alpha_- - \beta_+} e^{g_1/2} O(x^{-1/2})$$

$$= O\left(x^{\alpha} e^{\Im W/2 \sin(\varphi/2)}\right),$$

$$u_1(x; W) = x^{-\alpha_-} e^{-g_1/2} O(x^{-1/2})$$

$$= O\left(x^{-\alpha} e^{-\Im W/2 \sin(\varphi/2)}\right),$$

$$\alpha = 2^{-1} |\Im W|^{-1/2} \gamma_1 \sin(\varphi/2).$$

The obtained asymptotics are sufficient to allow definite conclusions on the deficiency indices of the initial symmetric operator $\hat{H}$ as functions of the parameters $g_1$, $g_2$ and thereby on a possible variety of its s.a. extensions. It is evident that for $\Im W > 0$, the function $u_1(x; W)$ exponentially increases at infinity and is not square-integrable. The function $u_1(x; W)$ 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 equation (4) is square-integrable at the origin). Because for $\Im W > 0$, the functions $u_1$, $v_1$ form a fundamental system of solution (4), this equation with $\Im W > 0$ 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 \( \hat{H} \). The structure of these extensions, in particular, the appearance of their specifying asymptotic boundary conditions, depends crucially on a specific range of values of the parameter \( g_2 \). In what follows, we identify five such regions and consider them separately.

3. Self-adjoint extensions and spectral analysis

3.1. The first range \( g_2 \geq 3/4 \) (\( \mu \geq 1 \))

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 \( D_{\hat{H}_1} = D_{\hat{H}}^* (\mathbb{R}_+) \) (5).

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

\[
(\hat{H} - W)\psi_\epsilon(x) = \eta(x), \quad \eta(x) \in L^2(\mathbb{R}_+),
\]

with \( \text{Im} W \neq 0 \) under the condition that \( \psi_\epsilon \in D_{\hat{H}}^* (\mathbb{R}_+) \), i.e. under the condition that \( \psi_\epsilon \) is square-integrable\(^5\), \( \psi_\epsilon(x) \in L^2(\mathbb{R}_+) \) (see [15, 16]). The general solution of this equation without the condition of square integrability can be represented as

\[
\psi_\epsilon(x) = a_1 u_1(x; W) + a_2 v_1(x; W) + I(x; W), \\
\psi_\epsilon^*(x) = a_1 u_1^*(x; W) + a_2 v_1^*(x; W) + I^*(x; W),
\]

where

\[
I(x; W) = \int_0^x G^{(\epsilon)}(x, y; W) \eta(y) \, dy \\
I^*(x; W) = \int_0^x d_1 G^{(\epsilon)}(x, y; W) \eta(y) \, dy
\]

\[
G^{(\epsilon)}(x, y; W) = \omega^{-1}(W) u_1(x; W) u_1(y; W), \\
G^{(\epsilon)}^*(x, y; W) = \omega^{-1}(W) u_1^*(x; W) v_1^*(y; W),
\]

with \( \omega \) 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 \( \psi_\epsilon(x) \in L^2(\mathbb{R}_+) \) 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 \( v_1(x; W) \)

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

Together with the fact that the functions \( \psi_\epsilon \) vanish at infinity (see below), this implies that the asymmetry form \( \Delta_{H^*} \) is trivial, which confirms that in the first range the operator \( H^* \) is symmetric and therefore s.a. (in contrast to the ranges considered in the subsequent sections).

It follows that Green’s function is given by

\[
G(x, y; W) = \begin{cases} 
G^{(\epsilon)}(x, y; W), & x > y, \\
G^{(\epsilon)}^*(x, y; W), & x < y.
\end{cases}
\]

The representation (9) of the function \( v_1 \) in terms of the functions \( u_1 \) and \( v_2 \) is inconvenient sometimes, because the individual summands do not exist for some \( \mu \) although \( v_1 \) does. For our purposes, other representations are convenient. For \( m - 1 < 2\mu < m + 1 \), \( m \geq 2 \), the function \( v_1(x; W) \) can be represented as

\[
v_1(x; W) = A_m(W) u_1(x; W) + \frac{\omega(W)}{2\mu} v_{(m)}(x; W), \\
A_m(W) = \frac{x^{2\mu} \Gamma(-2\mu) \Gamma(\alpha_m)}{\Gamma(\alpha_m)} + a_m(W) \frac{\Gamma(2\mu) \Gamma(\beta_m)}{\Gamma(\alpha_m)}, \\
v_{(m)}(x; W) = u_2(x; W) - a_m(W) \Gamma(\beta_m) u_1(x; W), \\
a_m(W) = \frac{x^{\mu} \Gamma(\alpha_m)}{m! \Gamma(\alpha_m - \nu_m)}, \quad \alpha_{\pm m} = \frac{1 \pm m}{2} + \frac{\nu_1}{\lambda}.
\]

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

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

(see [17, 18]), the functions \( u_{(m)}(x; W) \) and \( A_m(W) \) exist for \( m - 1 < 2\mu < m + 1 \) and for any \( W \). In fact, \( u_{(m)}(x; W) \) are particular solutions of equation (4), which are real-entire in \( W \) and have the properties (for \( m - 1 < 2\mu < m + 1 \))

\[
W \partial(u_1, u_{(m)}) = -2\mu, \quad u_{(m)}(x; W) = x^{1/2 - \mu} \tilde{O}(x), \quad x \to 0.
\]

As a guiding functional, we take

\[
\Phi(\xi; W) = \int_{\mathbb{D}} U(x; W) \xi(x) \, dx, \quad \xi \in D = D_1(\mathbb{R}_+) \cap D_{\hat{H}_s},
\]

where \( U(x; W) = u_1(x; W) \) and \( D_1(\mathbb{R}_+) \) is the space of arbitrary functions with a support bounded from the right: \( \Phi(x) \in D_1(\mathbb{R}_+) \Rightarrow \supp \Phi \subseteq [0, \beta], \beta < \infty \); 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 \( \xi \), the functional \( \Phi(\xi; W) \) is an entire function of \( W \); (2) if \( \Phi(\xi_0; \xi_0) = 0 \), \( \xi_0 \in \mathbb{D} \), then the inhomogeneous equation \( (\hat{H} - E_0)\psi = \xi_0 \) has a solution \( \psi \in \mathbb{D} \); (3) \( \Phi(\hat{H}\xi; W) = W \Phi(\xi; W) \). It is easy to verify
We thus find that for $g_1 > 0$, the generalized eigenfunctions $U_E(x) = \sqrt{\sigma(E)}u_1(x; E)$, $E \geq 0$, of $\hat{H}_1$ form a complete orthonormalized system in $L^2(\mathbb{R}_+^+)$. For $g_1 < 0$, the generalized eigenfunctions $U_E(x) = \sqrt{\sigma(E)}u_1(x; E)$, $E \geq 0$, of $\hat{H}_1$ together with the eigenfunctions $U_n(x) = Q_n u_1(x; E_n)$, $n \in \mathbb{Z}_+$, form a complete orthonormalized system in $L^2(\mathbb{R}_+^+)$. 

3.2. The second range $3/4 > g_2 > -1/4$, $g_2 \neq 0$

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, e.g., [12] and also [15, 16]), we begin by evaluating the quadratic asymptotic form $\Delta_{H^+}$ in terms of quadratic boundary forms, which are determined by the asymptotics of functions $\psi_\pm(x)$ belonging to the natural domain $D_{a^+}_b^\ast(\mathbb{R}_+)$ 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)\(^6\) (see [12]), and the asymptotic form $\Delta_{H^+}$ is reduced to (minus) the left boundary form. To determine the asymptotic behavior of functions $\psi_\pm(x)$ at the origin, we consider these functions as solutions of the inhomogeneous equation (14) with $W = 0$. Because, in the range under consideration, any solution of the homogeneous equation (4) is square-integrable at the origin, the general solution of equation (14) with $W = 0$ can be represented as

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

(23)

The asymptotic behavior for the functions $u_1$ and $u_2$ in the 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 that

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

(24)

With these asymptotics, we calculate the left boundary form $[\psi_\pm, \psi_\pm](0) = \lim_{x \to 0} \int (\psi_\pm(x)\psi_\pm^\ast(x) + \psi_\pm^\ast(x)\psi_\pm(x))$ and obtain a representation of the quadratic asymptotic form as a quadratic form in the coefficients $a_1$ and $a_2$ in (24):

$$
\Delta_{H^+}(\psi_\pm) = -2\mu k_0 (\tilde{a}_1 a_2 - \tilde{a}_2 a_1).
$$

\(\tilde{a}_1\) and $\tilde{a}_2$ are defined as

$$
\tilde{a}_1 = a_1 - \frac{1}{2\mu} \int_0^1 [u_1(x; 0)u_2(y; 0) - u_2(x; 0)u_1(y; 0)] \eta(y) \, dy,
$$

(25)

$$
\tilde{a}_2 = a_2 - \frac{1}{2\mu} \int_0^1 [u_1(x; 0)u_2(y; 0) - u_2(x; 0)u_1(y; 0)] \eta(y) \, dy.
$$

(26)

Moreover, we can prove that $\psi_\pm$ vanishes at infinity together with its derivative, $\psi_\pm(x), \psi_\pm^\ast(x) \to 0$ as $x \to \infty$.

The final result of this section is as follows.
The inertia indices of the quadratic form \( \psi \) satisfy relation \((25)\) with a fixed \( v \). These subspaces are just the domains of s.a. restrictions of \( S \) and relation \((25)\), with a fixed \( v \), defines the asymptotic boundary conditions specifying these s.a. operators.

We thus find that for each \( g_2 \) in the second range, there exists a family of s.a. Hamiltonians \( \tilde{H}_2 \) parametrized by the parameter \( v \) on a circle with the domains \( D_{\tilde{H}_2} \) and having the following asymptotic behavior as \( x \to 0 \):

\[
\psi(x) = C\psi^{\pm}(x) + O(x^{3/2}), \\
\psi'(x) = C\psi'^{\pm}(x) + O(x^{1/2}), \\
\psi^{\pm}(x) = u_{1\lambda}(k_0 x) v + \tilde{u}_{2\nu}(x, k_0) cos \nu.
\]

The spectral analysis of \( \tilde{H}_2 \) is similar to that for \( \tilde{H}_1 \) in the previous section, the difference being that the function \( v_1(x; W) \) is now square-integrable at the origin and we must take into account asymptotic boundary conditions \((26)\). To evaluate the Green’s function for \( \tilde{H}_2 \), we take the representation \((15)\) with \( a_1 = 0 \) for \( \psi_{\nu}(x) \) belonging to \( D_{\tilde{H}_2} \); boundary conditions \((26)\) and asymptotics \((11), (13a)\) then yield

\[
a_2 = k_0^{-2\mu} c^{-1} \left[ \Gamma(2\mu) / \Gamma(\alpha_1) \right]^{1/2} \cos \nu + \frac{\Gamma(-2\mu)(\lambda/k_0)^{2\mu}}{\Gamma(\alpha_1)} \cos \nu \right]^{-1} \\
\times \cos \nu \int_0^\infty v_1(x; W)\eta(\xi) dx.
\]

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

\[
v_1(x; W) = (2\mu)^{-1} k_0^{-1} c^{1/2+\nu} \omega(W) (\tilde{u}_{2\nu}(W) u_{2\nu}(x; W) \\
+ \tilde{u}_{2\nu}(W) \tilde{u}_{2\nu}(x; W)),
\]

\[
\tilde{u}_{2\nu}(W) = k_0^{1/2-\nu} u_1(x; W) \sin \nu + k_0^{-1/2-\nu} u_2(x; W) \cos \nu,
\]

\[
\tilde{u}_{2\nu}(W) = -k_0^{-1/2-\nu} u_1(x; W) \cos \nu + k_0^{1/2-\nu} u_2(x; W) \sin \nu,
\]

\[
\omega_{2\nu}(W) = \sin \nu + f(W) \cos \nu,
\]

\[
\tilde{\omega}_{2\nu}(W) = \cos \nu - f(W) \sin \nu,
\]

\[
f(W) = (\lambda/k_0)^{2\mu} \frac{\Gamma(\alpha_1)}{\Gamma(\alpha_1)},
\]

where \( \omega \) 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 equation \((4)\) and \( u_{2\nu}(x; W) \) satisfies boundary condition \((26)\), we obtain the

\[\text{Green's function}
\]

\[
G(x; y; W) = \Omega^{-1}(W) u_{2\nu}(x; W) u_{2\nu}(y; W) + \frac{1}{2\mu k_0} \left\{ (\tilde{u}_{2\nu}(x; W) u_{2\nu}(y; W), \quad x > y, \\
\tilde{u}_{2\nu}(y; W) u_{2\nu}(y; W), \quad x < y, \right. \]

\]

where

\[
\left. \Omega(W) = 2\mu k_0 \omega(W) \tilde{\omega}_{2\nu}^{-1}(W). \right)
\]

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 \( \xi \in \mathbb{D} = D_r(\mathbb{R}_+ \cap D_{\tilde{H}_2} \). The domain \( \mathbb{D} \) is dense in \( L^2(\mathbb{R}_+ \cap D_{\tilde{H}_2} \). 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 subsection 3.1. It is easy to verify the properties \((1)\) and \((3)\). We prove that the property \((2)\) also holds. Let

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

We consider the function

\[
\psi(x) = \frac{1}{2\mu k_0} \left[ u_{2\nu}(x; E_0) \int_x^b \tilde{u}_{2\nu}(y; E_0) \xi_0(y) dy + \tilde{u}_{2\nu}(x; E_0) \int_0^x u_{2\nu}(y; E_0) \xi_0(y) dy \right],
\]

which is a solution of equation

\[
(\tilde{H} - E_0) \psi(x) = \xi_0(x).
\]

Using condition \((29)\), we find that \( \psi \in [0, b] \), i.e. \( \psi \in D_r(\mathbb{R}_+ \cap D_{\tilde{H}_2} \), and therefore \( \psi \in L^2(c, b) \) for any \( c > 0 \).

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

\[
\psi(x) = c u_{2\nu}(x; E_0) + \tilde{u}_{2\nu}(x; E_0) \int_0^x u_{2\nu}(y; E_0) \xi_0(y) dy - u_{2\nu}(x; E_0) \int_0^x \tilde{u}_{2\nu}(y; E_0) \xi_0(y) dy,
\]

\[
c = \frac{1}{2\mu k_0} \int_0^b \tilde{u}_{2\nu}(y; E_0) \xi_0(y) dy.
\]

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 find that the asymptotic of \( \psi(x) \) at the origin is given by

\[
\psi(x) = c u_{2\nu}(x; E_0) + O(x^{5/2-\mu}), \quad x \to 0,
\]

which implies that \( \psi \in D_{\tilde{H}_2} \), and therefore \( \psi \in \mathbb{D} \).

The derivative of the spectral function reads

\[
\sigma'(E) = \pi^{-1} \text{Im } \Omega^{-1}(E + i0).
\]

It is convenient to consider the cases \( |v| < \pi/2 \) and \( v = \pm \pi/2 \) separately.
Finally, we consider the case \( \nu = \pi/2 \) where we have
\[
    u_{2, \pi/2}(x; W) = k_0^{1/2 - \mu} u_1(x; W),
\]
\[
    \Omega^{-1}(W) = - \frac{\Gamma(\alpha_+) \Gamma(\beta_-) (\lambda/k_0)^{2\mu}}{2\mu k_0 \Gamma(\alpha_-) \Gamma(\beta_+)}.
\]
We see that all results for the spectrum and system of the normalized (generalized) eigenfunctions coincide with those of the first range \((g_2 > 3/4)\). In particular, the expressions for discrete energy levels (we will denote them by \( \mathcal{E}_n \)) are given by equation (22):
\[
    \mathcal{E}_n = - \frac{g_1^2}{(1 + 2\mu + 2n)^2}, \quad \tau_n = \sqrt{|\mathcal{E}_n|} = \frac{|g_1|}{1 + 2\mu + 2n}.
\]
We obtain the same results for the case \( \nu = -\pi/2 \).

Secondly, we consider the case \( \nu = 0 \). Here we have
\[
    u_{2, 0}(x; W) = k_0^{1/2 - \mu} u_2(x; W),
\]
\[
    \sigma'(E) = \pi^{-1} \text{Im} \Omega^{-1}(E + i0),
\]
\[
    \Omega^{-1}(W) = \frac{(k_0/\lambda)^{2\mu} \Gamma(\beta_-) \Gamma(\alpha_-)}{2\mu k_0 \Gamma(\beta_+)}.
\]
We let \( g_1 > 0 \). For \( E = p^2 \geq 0, \quad p \geq 0, \quad \lambda = 2p e^{-i\pi/2} \), we have
\[
    \sigma'(E) = \left( \frac{\Gamma(\alpha_-)}{\Gamma(\beta_-)} \right)^2 \frac{(k_0/2p)^{2\mu} e^{-\pi\beta_+/2p}}{2\pi k_0}.
\]
For \( E = -r^2 < 0, \quad \tau > 0, \quad \lambda = 2\tau, \) the function \( \Omega^{-1}(E) \) is real in the case of those \( E \) for which \( \Omega^{-1}(E) \) is finite, such that \( \text{Im} \Omega^{-1}(E + i0) \) can differ from zero only for \( E \) that provide \( \Omega^{-1}(E) = \infty \). The latter is possible only for \( \alpha_- = -n \) \((\Gamma(\alpha_-) = \infty)\), \( n \in \mathbb{Z}^*_+ \), or
\[
    1 - 2\mu + g_1/\tau = -2n, \quad n \in \mathbb{Z}^*_+.
\]
Equation (32) has no solutions for \( 0 < \mu < 1/2 \) and has one solution for \( 1/2 < \mu < 1 \): \( n = 0, \quad \tau = \tau_1(0) = g_1/(2\mu - 1), \quad E = E_{-1}(0) = -\tau_1^2(0) \).

We now let \( g_1 < 0 \). For \( E = p^2 \geq 0, \quad p \geq 0, \quad \lambda = 2p e^{-i\pi/2} \), the derivative of the spectral function is given by equation (31).

For \( E = -r^2 < 0, \quad \tau > 0, \quad \lambda = 2\tau, \) the function \( \Omega^{-1}(E) \) is real for \( E \neq E_{n}(0) \) \((\Omega(E_{n}(0)) = \infty)\), such that \( \sigma'(E) \) does not vanish only in the points \( E = E_{n}(0) \). The equation \( \Omega^{-1}(E_{n}(0)) = \infty \) implies the condition \( \alpha_- = 1/2 - \mu = |g_1|/2\tau_n(0) = -n \) \((\Gamma(\alpha_-) = \infty)\), which gives
\[
    E_{n}(0) = -\tau_n^2(0) = -\left( \frac{g_1}{1 + 2\mu + 2k} \right)^2, \quad k = \left\{ \begin{array}{l}
    n, \quad 0 < \mu < 1/2, \\
    n + 1, \quad 1/2 < \mu < 1, 
\end{array} \right. n \in \mathbb{Z}^*_+.
\]
Thus, for \( g_1 < 0 \), the simple spectrum of \( \hat{H}_{2,0} \) is given by \( \operatorname{spec} \hat{H}_{2,0} = \mathbb{R} \cup \{ E_{n}(0), \quad n \in \mathbb{Z}^*_+ \} \) and a complete orthonormalized system in \( L^2(\mathbb{R}^+) \) consists of (generalized) eigenfunctions
\[
    U_E(x) = \sqrt{\sigma(E)} u_2(x; E), \quad E \geq 0,
\]
\[
    U_n(x) = \frac{(2\tau_0)^{-\mu}}{|\Gamma(\beta_-)|} \left( \frac{\Gamma(-2\mu + k)}{1 - 2\mu + 2k} \right)^{1/2} u_3(x; E_n(0)), \quad n \in \mathbb{Z}^*_+.
\]

of \( \hat{H}_{2,0} \).

For \( 0 < \mu < 1/2, \quad g_1 > 0 \), the simple spectrum of \( \hat{H}_{2,0} \) is given by \( \operatorname{spec} \hat{H}_{2,0} = \mathbb{R} \cup \{ E_{-1}(0) \} \) and a complete orthonormalized system in \( L^2(\mathbb{R}^+) \) consists of generalized eigenfunctions \( U_E(x) \) with the corresponding parameters and the function \( \sigma'(E) \).

Now, we turn to the general case \( |\nu| < \pi/2 \). In this case, we have
\[
    \sigma'(E) = \left( \frac{\Gamma(\alpha_-)}{\Gamma(\beta_-)} \right)^2 \frac{(k_0/2p)^{2\mu} e^{-\pi\beta_+/2p}}{2\pi k_0}.
\]
For \( E = p^2 \geq 0, \quad p \geq 0, \quad \lambda = 2p e^{-i\pi/2} \), we have
\[
    \sigma'(E) = \frac{B(E)}{2\pi k_0 \cos^2 \nu [A^2(E) + \mu^2 B^2(E)]},
\]
where \( A(E) = \text{Re} f_\nu(E) \) and \( \mu B(E) = -\text{Im} f_\nu(E) \). A direct calculation gives
\[
    A(E) = \frac{\mu |\Gamma(\alpha_-)|^2 (2p/k_0)^{2\mu}}{\Gamma^2(\beta_-)} \left( e^{-\pi\beta_+/2p} \cos(2\mu \pi) + e^{\pi\beta_+/2p} \right) + \tan \nu,
\]
\[
    B(E) = \frac{|\Gamma(\alpha_-)|^2 (2p/k_0)^{2\mu} e^{-\pi\beta_+/2p}}{\Gamma^2(\beta_-)}.
\]
For \( E = -r^2 < 0, \quad \tau > 0, \quad \lambda = 2\tau, \) the function \( f_\nu(E) \) is real; therefore, \( \sigma'(E) \) can differ from zero only at the discrete points \( E_n(\nu) \) such that \( f_\nu(E_n(\nu)) = 0 \), or \( f(E_n(\nu)) = -\tan \nu \), and we find that (derivatives with respect to \( E \) are denoted by primes in equation (36))
\[
    \sigma'(E) = \sum_n \left[ -2\mu k_0 f'_\nu(E_n(\nu)) \cos^2 \nu \right]^{-1} \delta(E - E_n(\nu)),
\]
\[
    f'_\nu(E_n(\nu)) = f'(E_n(\nu)) < 0, \quad \delta_n(E_n(\nu))
\]
\[
    = -\cos^2 \nu \left[ f'(E_n(\nu)) \right]^{-1} > 0.
\]

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Because $f'(E_n(v)) < 0$ (see equation (36)), the straight line $f(E) = \tan v$, $E \in (-\infty, 0)$, can intersect the plot of the function $f'(E)$ not more than once. That is why the equation $f(E) = 0$ has no solutions for $v \in (v_{-1}, \pi/2)$, whereas for any fixed $v \in (-\pi/2, v_{-1}]$, this equation has only one solution $E_{-1}(v) \in (-\infty, 0)$, which increases monotonically from $-\infty$ to $0$ as $v$ changes from $-\pi/2 + 0$ to $v_{-1}$.

We thus find that the spectrum of $\tilde{H}_{2,v}, |v| < \pi/2$, with $g_1 > 0$, is simple and is given by

$$\text{spec} \tilde{H}_{2,v} = \begin{cases} \mathbb{R}_+ \cup \{E_{-1}(v)\}, & v \in (-\pi/2, v_{-1}], \\ \mathbb{R}_+, & v \in (v_{-1}, \pi/2). \end{cases}$$

The generalized eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} u_{2,v}(x; E), \quad E > 0,$$

and (for $v \in (-\pi/2, v_{-1}]$) the eigenfunction

$$U_{-1}(x) = \left[ -2\mu k_0 f'(E_{-1}(v)) \cos^2 v \right]^{-1/2} u_{2,v}(x; E_{-1}(v))$$

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

II. Let $g_1 < 0$.

Then for $E = p^2 > 0$, $p > 0$, $\lambda = 2p \sqrt{e^{-\tau/2}}$, formulae (34) and (35) hold true. Because the functions $A(E)$ and $B(E)$ are finite at $E = 0$ ($B(0) \neq 0$), the function $\sigma'(E)$ (34) is a finite positive function for $E > 0$. This means that for $E > 0$, the spectra of s.a. Hamiltonians $\tilde{H}_{2,v}$ are simple, purely continuous, and given by $\text{spec} \tilde{H}_{2,v} = \mathbb{R}_+$.

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

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

It is easy to see that for fixed $v$, the spectrum is bounded from below and the equation $f(E_n(v)) = 0$ has an infinite number of solutions

$$E_n(v) = -g_1^2/4n^2 + O(n^{-3}),$$ (37)

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

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

$$U_E(x) = \sqrt{\sigma'(E)} u_{2,v}(x; E), \quad E > 0,$$

and eigenfunctions of the discrete spectrum

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

of $\tilde{H}_{2,v}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. It is possible to present a description of the discrete spectrum of the Hamiltonians $\tilde{H}_{2,v}, |v| < \pi/2, g_1 < 0$ in more detail.

The function $f(E)$ has the properties $f(E) \to \infty$ as $E \to -\infty$; $f(E_n(0)) = \pm \infty$, $n \in \mathbb{Z}_+$, and we have

$$E_n(0) < E_n < E_{n+1}(0) < E_{n+1}, \quad n \in \mathbb{Z}_+.$$  

Taking into account the third equality in (36), we can see that in each energy interval $(E_n, E_{n+1})$, $n \in \mathbb{Z}_+$, for a fixed $v \in (-\pi/2, \pi/2)$, there is one discrete level $E_n(v)$ that increases monotonically from $E_{n+1}(0)$ to $E_n(0)$ when $v$ changes from $\pi/2$ to $-\pi/2 + 0$ (we set $E_{-1} = -\infty$). We note that the relations

$$\lim_{v \to \pi/2} E_n(v) = \lim_{v \to -\pi/2} E_{n+1}(v) = E_n, \quad n \in \mathbb{Z}_+$$

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

It should also be pointed out that bound states exist even for the repulsive potential, $g_2, g_1 > 0$; see the dashed line in 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 $\alpha_1 = \alpha_2 = \alpha = 1/2 + g_1/\lambda$, $\beta_+ = \beta_- = 1$, $u_1(x; W) = u_2(x; W)$, and the representation (9) of $\psi_1(x; W)$ in terms of $u_1$ and $u_2$ does not hold. As the solutions of equation (4) with $g_2 = -1/4$, we therefore use
the functions \( u_1(x; W) \), \( u_3(x; W) \) and \( \upsilon_1(x; W) \), respectively defined by
\[
\begin{align*}
  u_1(x; W) &= x^{1/2} e^{-\gamma x/2} \Phi(\alpha, 1; z) = u_1(x; W)|_{x \to -\gamma}, \\
  u_3(x; W) &= \frac{\partial}{\partial \mu} \left[u_1(x; W)|_{\mu = 0} + \ln k_0 u_1(x; W), \right] \\
  \upsilon_1(x; W) &= x^{1/2} e^{-\gamma x/2} \Psi(\alpha, 1; z) \\
  = (1-\gamma) (\omega_0(W) u_1(x; W) - u_3(x; W)), \\
  \omega_0(W) &= 2 \psi(1) - \psi(\alpha) - \ln(\lambda/k_0),
\end{align*}
\]
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
\[
\begin{align*}
u_1(x; W) &= k_0^{-1/2} u_{1a}(x) + O(x^{1/2}), \\
 u_{1a}(x) &= (x^{1/2}), \\
 u_3(x; W) &= k_0^{-1/2} u_{3a}(x) + O(x^{3/2} \ln x), \\
 u_{3a}(x) &= (x^{1/2} \ln(k_0 x)), \\
 \upsilon_1(x; W) &= k_0^{-1/2} (1-\gamma) (\omega_0(W) u_{1a}(x) \\
 - u_{3a}(x)) + O(x^{3/2} \ln x).
\end{align*}
\]
As \( x \to \infty \), \( \Im W > 0 \), we have
\[
\begin{align*}
u_1(x; W) &= \Gamma(1-\gamma)(\lambda^{1-\gamma} x^{1/2} \hat{\vartheta}(x^{-1}) \to \infty, \\
 \upsilon_1(x; W) &= \lambda^{-\gamma} x^{-1/2} \hat{\vartheta}(x^{-1}) \to 0.
\end{align*}
\]
Both sets \( u_1, u_3 \) and \( \upsilon_1, \upsilon_1 \) are linearly independent, \( \text{Wr}(u_1, u_3) = 1 \), \( \text{Wr}(u_1, \upsilon_1) = -\Gamma(1-\gamma) \), and in particular, \( u_1 \) and \( \upsilon_1 \) form a fundamental system of solutions of equation (4) for \( \Im W \neq 0 \) and \( W = 0 \); see section 2.

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 section 2.

To evaluate the asymptmetry form in terms of a.b. coefficients, we need to determine the asymptotics of functions \( \psi_\sigma \) belonging to the natural domain \( D^*_\sigma(\mathbb{R}_+) \) at the origin. To this end, we use the general solution (23) of equation (14), performing there the substitutions \( a_{2\mu} = a_{2\mu} \) and \( a_{3\mu} / 2\mu \to -a_{3\mu} \).

Taking into account that the potential vanishes as \( x \to \infty \), we have \( \psi_\sigma(x), \psi_\sigma'(x) \to 0 \). Using the Cauchy–Bunyakovskii inequality to estimate the integral terms, we find that the desired asymptotic as \( x \to 0 \) is given by
\[
\begin{align*}
  \psi_\sigma(x) &= a_1 u_{1a}(x) + a_2 u_{3a}(x) + O(x^{1/2} \ln x), \\
  \psi_\sigma'(x) &= a_1 u_{1a}'(x) + a_2 u_{3a}'(x) + O(x^{1/2} \ln x).
\end{align*}
\]
Then we find that \( \Delta_{H}\sigma \) vanishes results in the relation
\[
a_1 \cos \vartheta = a_2 \sin \vartheta, \quad \vartheta \in \mathbb{S}(-\pi/2, \pi/2).
\]
Thus, there exists a family of s.a. Hamiltonians \( \hat{H}_{3,\vartheta} \) with the domains \( D_{H,\sigma} \) that consist of functions from \( D^*_\sigma(\mathbb{R}_+) \) with the following asymptotic behavior as \( x \to 0 \):
\[
\begin{align*}
  \psi &= C \psi_{3,\sigma}(x) + O(x^{1/2} \ln x), \\
  \psi' &= C \psi'_{3,\sigma}(x) + O(x^{1/2} \ln x), \\
  \psi_{3,\sigma}(x) &= \psi \cos \vartheta + u_{3a}(x) \sin \vartheta.
\end{align*}
\]
Therefore,
\[
D_{H,\sigma} = \left\{ \psi : \psi \in D^*_\sigma(\mathbb{R}_+), \psi \ obey (40) \right\}.
\]
Imposing s.a. boundary condition (40) on the functions (15) (with \( a_1 = 0 \), and using asymptotics (38), we find the Green’s functions of the operators \( \hat{H}_{3,\vartheta} \):
\[
\begin{align*}
  G(x, y; W) &= \Omega^{-1}(W) u_{3,\sigma}(x; W) u_{3,\sigma}(y; W) \\
  &= \psi_{3,\sigma}(x; W) u_{3,\sigma}(y; W), \quad x > y, \\
  &= u_{3,\sigma}(x; W) u_{3,\sigma}(y; W), \quad x < y,
\end{align*}
\]
where
\[
\begin{align*}
  \Omega(W) &= (\omega_0 \cos \vartheta + \sin \vartheta) (\omega_0 \sin \vartheta - \cos \vartheta)^{-1}, \\
  u_{3,\sigma}(x; W) &= u_1(x; W) \sin \vartheta + u_3(x; W) \cos \vartheta, \\
  \bar{u}_{3,\sigma}(x; W) &= u_1(x; W) \cos \vartheta - u_3(x; W) \sin \vartheta, \\
  \Gamma(\alpha) u_1 &= (\omega_0 \sin \vartheta - \cos \vartheta) u_{3,\sigma} + (\omega_0 \cos \vartheta + \sin \vartheta) \bar{u}_{3,\sigma}.
\end{align*}
\]
We note that \( u_{3,\sigma} \) and \( \bar{u}_{3,\sigma} \) are solutions of equation (4) real-entire in \( W \), the solution \( u_{3,\sigma} \) satisfies the boundary condition (40) and 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 \( U = u_{3,\sigma} \) satisfies the properties (1) and (3) cited in section 3.1. The proof that it satisfies the property (2) is identical to that presented in section 3.2 for the second range \( 1 > \mu > 0 \). It follows that the spectra of \( H_{3,\vartheta} \) are simple.

The derivative of the spectral function is given by
\[
\sigma'(E) = \pi^{-1} \Im \Omega^{-1}(E + i0),
\]
We first consider the case \( \vartheta = \pi/2 \), where we have
\[
\begin{align*}
  u_{3,\pi/2}(x; W) &= u_1(x; W), \quad \Omega(W) = -[\psi(\alpha) + \ln(\lambda/k_0)]^{-1}. \\
  \text{For} \quad E = p^2 \geq 0, \quad p \geq 0, \quad \lambda = 2p e^{-i\pi/2}, \quad \text{we find that} \\
  \sigma'(E) &= \frac{1}{2} \left( 1 - \tanh \frac{\pi R_1}{2p} \right) \geq 0.
\end{align*}
\]
For \( E = -\tau^2 < 0, \quad \tau > 0, \quad \lambda = 2\tau \), and \( g_1 > 0 \), the function \( \Omega(E) \) is of the form
\[
\Omega(E) = -[\psi(1/2 + g_1/2\tau) + \ln(2\tau/k_0)]^{-1},
\]
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
\[
\Omega(E) = -[\psi(1/2 - |g_1|/2\tau) + \ln(2\tau/k_0)]^{-1},
\]
which implies that there are discrete negative energy levels $E_n$ in the spectrum,
\[
E_n = -g_1^2(1 + 2n)^{-2}, \quad \tau_n = |g_1|(1 + 2n)^{-1}, \quad n \in \mathbb{Z}.
\]
\[
\sigma'(E) = \sum_{n \in \mathbb{Z}} Q_n^2 \delta(E - E_n), \quad Q_n = 2|g_1|(1 + 2n)^{-3/2}.
\]

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

We thus find that for $g_1 > 0$, the spectrum of $\hat{H}_{3,\pi/2}$ is simple, given by $\hat{H}_{3,\pi/2} = \mathbb{R}_+$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its generalized eigenfunctions is
\[
U_E(x) = \sqrt{\sigma'(E)} u_1(x; E), \quad E \geq 0.
\]
For $g_1 < 0$, the spectrum of $\hat{H}_{3,\pi/2}$ is simple and is given by $\hat{H}_{3,\pi/2} = \mathbb{R}_+ \cup \{ E_n, n \in \mathbb{Z} \}$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions consists of functions
\[
U_E(x) = \sqrt{\sigma'(E)} u_1(x; E), \quad E \geq 0,
\]
\[
U_n(x) = 2|g_1|(1 + 2n)^{-3/2} u_1(x; E_n), \quad E_n < 0.
\]
We note that the spectrum and eigenfunctions for $\hat{H}_{3,\pi/2}$ coincide with those for $\hat{H}_1$ with $g_2 \geq 3/4$ if we set $\mu = 0$ in the respective formulae in section 3.1. We now turn to the case $|\vartheta| < \pi/2$. In this case, $\sigma'(E)$ can be represented as
\[
\sigma'(E) = (\pi \cos^2 \vartheta)^{-1} \text{Im}[\omega_3(E + i0)]^{-1},
\]
\[
\omega_3(W) = \psi(\alpha) + \ln(\lambda/k_0) - 2\psi(1) - \tan \vartheta.
\]
For $E = p^2 \geq 0$, $p > 0$, $\lambda = 2p e^{-\pi/2}$ and $g_1 < 0$, we have
\[
\sigma'(E) = \frac{B(E)}{\pi \cos^2 \vartheta [A^2(E) + B^2(E)]},
\]
where $\omega_3(E) = A(E) - iB(E)$. The function $B(E)$ can be explicitly calculated:
\[
B(E) = \frac{\pi}{2} \left[ 1 - \tan \vartheta \frac{g_1}{2\sqrt{E}} \right] > 0, \quad \forall E \geq 0,
\]
whence it follows that for all $E \geq 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is purely continuous.

For $E = p^2 > 0$, $p > 0$, $\lambda = 2p e^{-\pi/2}$ and $g_1 > 0$, the spectral function is given by the same equations (41) and (42). But in this case, $B(0) = 0$ and the limit $\lim_{E \to \vartheta} \omega_3(W)$ must be carefully examined.

At small $W$, we have
\[
\omega_3(W) = (\tan \vartheta) - \vartheta - (6g_1^2)^{-1} W + \mathcal{O}(W^2),
\]
\[
\tan \vartheta = \ln(g_1/k_0) - 2\psi(1).
\]

For $\vartheta \neq \vartheta(-)$, the function $\sigma'(E)$ is finite at $E = 0$. But for $\vartheta = \vartheta(-)$ and small $E$, we have
\[
\sigma'(E) = -\frac{6g_1^2}{\pi \cos^2 \vartheta} \delta(E + i0) + \mathcal{O}(1)
\]
\[
= -\frac{6g_1^2}{\cos^2 \vartheta} \delta(E) + \mathcal{O}(1),
\]
which means that the spectrum of the Hamiltonian $\hat{H}_{3,\vartheta(-)}$ 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 $E_n = E_\vartheta(\vartheta)$ of $\omega_3(E)$, which yields
\[
\sigma'(E) = \sum_n \left[ -k_0 \omega_3'(E_n(\vartheta)) \cos^2 \vartheta \right]^{-1} \delta(E - E_n(\vartheta)),
\]
\[
\omega_3(E_n(\vartheta)) = 0, \quad \omega_3'(E_n(\vartheta)) < 0,
\]
and
\[
\partial_\vartheta E_n(\vartheta) = \left[ \cos^2 \vartheta \omega_3'(E_n(\vartheta)) \right]^{-1} < 0.
\]

For $g_1 > 0$, we have
\[
\omega_3(E) = \psi(1/2 + g_1/2\tau) + \ln(2\tau/k_1) + \tan \vartheta - \tan \vartheta,
\]
\[
\omega_3(E) = (1/2) \ln \left| E - \tan \vartheta + \mathcal{O}(1), \quad E \to -\infty, \right.
\]
\[
\omega_3(0) = \tan \vartheta - \tan \vartheta.
\]

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

For $g_1 < 0$, we have
\[
\omega_3(E) = \psi(1/2 - |g_1|/2\tau) + \ln(2\tau/k_1) - 2\psi(1) - \tan \vartheta,
\]
\[
\omega_3(E) = (1/2) \ln \left| E - \tan \vartheta + \mathcal{O}(1), \quad E \to -\infty, \right.
\]
\[
\omega_3(0) = \tan \vartheta - \tan \vartheta.
\]

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 $n \to \infty$, $E_n = -g_1^2/4n^2 + \mathcal{O}(1/n^3)$.

We thus find that for $g_1 > 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is simple and is given by $\hat{H}_{3,\vartheta} = \mathbb{R}_+ \cup \{ E^{(-)}(\vartheta) \}$ and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions consists of functions
\[
U_E(x) = \sqrt{\sigma'(E)} u_{1,\vartheta}(x; E), \quad E \geq 0,
\]
\[
U_n(x) = \left[ -k_0 \cos^2 \vartheta \omega_3'(E_n(\vartheta)) \right]^{-1/2} u_{3,\vartheta}(x; E^{(-)}(\vartheta))
\]
(the eigenvalue $E^{(-)}(\vartheta)$ exists and therefore $E^{(-)}(\vartheta)$ and the corresponding eigenfunction $U(x)$ enter the inversion formulae only if $\vartheta \geq \vartheta(-)$); for $g_1 < 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is simple and is given by $\hat{H}_{3,\vartheta} = \mathbb{R}_+ \cup \{ E_n \}$ and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions consists of the functions
\[
U_E(x) = \sqrt{\sigma'(E)} u_{1,\vartheta}(x; E), \quad E \geq 0,
\]
\[
U_n(x) = \left[ -k_0 \cos^2 \vartheta \omega_3'(E_n(\vartheta)) \right]^{-1/2} \times u_{3,\vartheta}(x; E_n(\vartheta)), \quad E_n(\vartheta) < 0.
\]
It is possible to describe the discrete spectrum for $|\theta| < \pi/2$ and $g_1 < 0$ in more detail. To this end, we represent the equation $\omega_\beta(E(\theta)) = 0$ in the equivalent form
\[ f(E) = \tan \theta, \quad f(E) = \psi(1/2 - |\theta_1|/2\tau) + \ln(2\tau/k_0) - 2\psi(1). \]

Then we have
\[ f(-\infty) = \infty, \quad f(\mathcal{E}_n \pm 0) = \pm \infty, \quad n \in \mathbb{Z}_+. \]

Because equation (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 $E_n(\theta)$ and $E_n(\theta)$ increases monotonically from $\mathcal{E}_n \pm 0$ to $\mathcal{E}_{n+1} - 0$ when $\theta$ changes from $\pi/2 - 0$ to $-\pi/2 + 0$ (we set $\mathcal{E}_{-1} = -\infty$). We note the relations
\[ \lim_{\theta \to -\pi/2} E_{n-1}(\theta) = \lim_{\theta \to -\pi/2} E_n(\theta) = \mathcal{E}_n. \]

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

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

According to section 2, the deficiency indices of the initial symmetric operator $\hat{H}$ with $g_2 < -1/4$ are $m_1 = 1$ and therefore there exists a one-parameter family of its s.a. extensions.

To evaluate the asymmetry form $\Delta_{H_{\psi}}$, we determine the asymptotics of functions $\psi_n$ belonging to $D^*_{\hat{H}}(\mathbb{R}_+)$ at the origin using representation (23) with $\mu = i\kappa$ of the general solution of equation (14) with $W = 0$ and estimating the integral terms by means of the Cauchy–Bunyakovskii inequality; we find that as $x \to 0$,
\[ \psi_n(x) = a_1 u_{1a}(x) + a_2 u_{2a}(x) + O(x^{3/2}), \]
\[ \psi'(x) = a_1 u'_{1a}(x) + a_2 u'_{2a}(x) + O(x^{1/2}), \]
\[ u_{1a}(x) = (k_0 x)^{1/2+i\kappa}, \quad u_{2a}(x) = (k_0 x)^{1/2-i\kappa} = u_{1a}(x). \]

Thus, we find that $\Delta_{H_{\psi}}(\psi_n) = -2i\kappa(\tau_0^1 \tau_1^2 - \tau_1^1 \tau_0^2)$, which means that the deficiency indices of $H_{\psi}$ are $m_1 = 1$. The condition $\Delta_{H_{\psi}}(\psi_n) = 0$ yields $a_1 = e^{i\phi_1} a_2$, $\theta \in [0, \pi)$.

Therefore, there exists a family of s.a. Hamiltonians $\hat{H}_{4,\rho}$ with the domains $D_{\hat{H}_{4,\rho}}$ that consist of functions from $D^*_{\hat{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:
\[ \psi = C \psi_{4a}(x) + O(x^{3/2}), \quad \psi' = C \psi'_{4a}(x) + O(x^{1/2}), \]
\[ \psi_{4a}(x) = e^{i\phi} u_{1a}(x) + e^{-i\phi} u_{2a}(x) = \psi_{2a}(x). \]

Therefore,
\[ D_{\hat{H}_{4,\rho}} = \left\{ \psi : \psi \in D^*_{\hat{H}}(\mathbb{R}_+), \psi \text{ obey (44)} \right\}. \]

Imposing the s.a. boundary condition (44) on the functions (15) (with $a_1 = 0$), and using asymptotics (11), we obtain the Green’s function of the operators $\hat{H}_{4,\rho}$.
\[ G(x, y; W) = \Omega^{-1}(W) u_{4,\rho}(x; W) u_{4,\rho}(y; W) \]
\[ - \frac{1}{4\kappa k_0} \left[ \tilde{a}_{4,\rho}(x; W) u_{4,\rho}(y; W), \quad x > y, \right. \]
\[ \left. u_{4,\rho}(x; W) \tilde{a}_{4,\rho}(y; W), \quad x < y, \right. \]

where
\[ \Omega(W) = \frac{4i\kappa k_0 \omega_{4,\rho}(W)}{\omega_{4,\rho}(W)}, \quad \omega_{4,\rho}(W) = a(W) + b(W), \]
\[ \tilde{a}_{4,\rho}(W) = a(W) - b(W), \quad a(W) = e^{i\phi} \frac{\Gamma(\beta)(\lambda/k_0)^{-i\kappa}}{\Gamma(\alpha)}, \]
\[ b(W) = e^{-i\phi} \frac{\Gamma(\beta)(\lambda/k_0)^{i\kappa}}{\Gamma(\alpha)}, \]
\[ u_{4,\rho}(x; W) = e^{i\phi} k_0^{1/2+i\kappa} u_1(x; W) + e^{-i\phi} k_0^{1/2-i\kappa} u_2(x; W), \]
\[ \tilde{a}_{4,\rho}(x; W) = i[e^{-i\phi} k_0^{1/2-i\kappa} u_2(x; W) - e^{i\phi} k_0^{1/2+i\kappa} u_1(x; W)], \]
\[ 4\kappa V_1(x; W) = - \frac{\lambda(k_0)^{-i\kappa}}{k_0^{1/2+i\kappa}}[\omega_{4,\rho}(W) u_{4,\rho}(x; W) + \omega_{4,\rho}(W) V_0(x; W)]. \]

where $u_{4,\rho}$ and $\tilde{a}_{4,\rho}$ are real-entire in $W$ solutions of equation (4), the solution $u_{4,\rho}$ satisfies boundary conditions (44), and the second term in $G(x, y; W)$ is real for real $W = E$.

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

The derivative of the spectral function has the form
\[ \sigma'(E) = \pi^{-1} \mathrm{Im} \Omega^{-1}(E+0). \]

For $E = p^2 > 0$, $p > 0$, $\lambda = 2p e^{-i\pi/2}$, and $g_1 < 0$, we have
\[ \sigma'(E) = \pi^{-1} \mathrm{Im} \Omega^{-1}(E) = \frac{(4\pi k_0)^{-1} (1-|D(E)|^2)}{(1+D(E))(1+D(E))}, \]

\[ D(E) = \frac{a(E)}{b(E)} = e^{-2\phi} \frac{\Gamma(\beta)(\pi/\beta)^e^{i\phi} \ln(k_0^2/2\rho)}{\Gamma(\beta)(\pi/\beta)} e^{-\pi x}. \]

Because
\[ |D(E)|^2 = 1 + e^{-2\pi x} e^{-\pi x} e^{\pi x} < 1, \quad \forall p \geq 0, \]

we have the $\hat{H}_{4,\rho} = \mathbb{R}_+$.

For $E = p^2 > 0$, $p > 0$, $\lambda = 2p e^{-i\pi/2}$, and $g_1 > 0$, expressions (45) and (46) for $\sigma'(E)$ hold true. But in this case, we have $|D(0)| = 1$ and must carefully examine the limit $\lim_{E \to 0+} \Omega^{-1}(W)$.

It is easy to see that for small $W$, we have the representation
\[ \Omega^{-1}(W) = - \frac{1}{4\kappa k_0} \frac{1 + e^{2i(\theta_0 - \theta)}}{[1 - e^{2i(\theta_0 - \theta)}] + iW/A + O(1)}, \]
\[ A = \frac{3\kappa^2}{\kappa(1+4\kappa^2)}, \]
\[ \theta_0 = \varphi - \pi([\varphi/\pi] + 1), \]
\[ \varphi = \pi \ln(k_1/k_0) - \theta + \pi/2, \]
\[ \theta_1 = \frac{1}{2} \ln \frac{\Gamma(\beta)}{\Gamma(\beta)}, \]

where $[\varphi/\pi]$ is the entire part of $\varphi/\pi$. For $\theta \neq \theta_0$, the function $\sigma'(E)$ is finite at $E = 0$. But for $\theta = \theta_0$, we find that
\[ \sigma'(E+0) = - \pi^{-1} (A/2\pi k_0) \mathrm{Im} (E+0)^{-1} + O(1) \]
\[ = (A/2\pi k_0) \delta(E) + O(1), \]
which means that the spectrum of the Hamiltonian $\hat{H}_{a,b}$ with $g_1 > 0$ contains the eigenvalue $E = 0$.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\Omega(E)$ can be represented as

$$\Omega(E) = [\pi \tan \theta(E)]^{-1},$$

$$\Theta(E) = \theta + \theta_0 - \theta_1(E) + \pi \ln(k_0/\tau),$$

where

$$\theta_1(E) = \frac{1}{2i} \left[ \ln \Gamma(1/2 + g_1/\tau + ix) - \ln \Gamma(1/2 + g_1/\tau - ix) \right]$$

$$+ \frac{-\pi |g_1|/\tau + \pi \ln(|g_1|/\tau) + O(1), \quad g_1 < 0}{\pi \ln(g_1/\tau) + O(\tau), \quad g_1 > 0, \quad E \to 0,}$$

$$\theta_1(-\infty) = \frac{1}{2i} \ln \Gamma(1/2 + ix) + O(1/\tau), \quad E \to -\infty.$$  

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

$$\Theta(E) = \begin{cases} \frac{\pi |g_1|/2 + \pi (1 + O(1)), \quad g_1 < 0,} \theta + \theta_1 - \pi \ln(k_0/\tau) + O(1/\tau), \quad g_1 > 0, \quad E \to 0,} 
\theta_1(-\infty) + \pi \ln(k_0/\tau) + O(1/\tau), \quad E \to -\infty. \end{cases}$$

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

$$\sigma'(E) = \sum_n Q_n^2 \delta(E - E_n(\theta)), \quad Q_n = \left|4\pi k_0^2 \Theta'(E_n(\theta))\right|^{-1/2},$$

$$\Theta'(E_n(\theta)) > 0.$$  

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

$$f(E) = \pi/2 + \pi (n - \theta/\pi),$$

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

we find 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 $\theta$ 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: $E_n(\theta) \to -\infty$ as $n \to -\infty$.

(c) For any $\theta$, the negative part of the spectrum is of the form $E_n(\theta) = -k_0^2 m^2 \tau^2 |n|/\pi (1 + O(1/n))$ 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 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 $E_n(\theta) = -k_0^2 m^2 \tau^2 |n|/\pi (1 + O(1/n^2))$ 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, $n \leq n_{max}$, where

$$n_{max} = \begin{cases} n_0 \quad \text{if} \quad f(0)/\pi - 1/2 = n_0, \quad 0 \leq \theta < \pi, \\ n_0 + 1 \quad \text{if} \quad f(0)/\pi - 1/2 > n_0, \quad 0 \leq \theta < \theta_0, \end{cases},$$

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

The final result is as follows: the spectrum of $\hat{H}_{a,b}$ is simple and given by

$$\text{spec } \hat{H}_{a,b} = \mathbb{R} \cup \{E_n \leq 0, \quad -\infty < n < n_{max}\},$$

where $n_{max} < \infty$ for $g_1 > 0$ and $n_{max} = \infty$ for $g_1 < 0$, and the set of corresponding (generalized) eigenfunctions

$$U_E(x) = \sqrt{\pi} \epsilon^{E \pi} u_{a,b}(x; E), \quad E \geq 0,$$

$$U_n(x) = Q_n u_{a,b}(x; E_n(\theta)), \quad E_n(\theta) \leq 0,$$

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

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

The analysis in this section is similar to that in section 3.2. A peculiarity is that the function $n_2$ is not defined for $\mu = 1/2$, and we therefore use the following solutions of equation (4):

$$u_1(x; W) = x e^{-x/2} \Phi(\alpha_{1/2}, 2; z),$$

$$u_5(x; W) = \tilde{u}_5(x; W) - g_1 \ln k_0 u_4(x; W),$$

$$u_1(x; W) = x e^{-x/2} \Phi(\alpha_{1/2}, 2; z),$$

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

where

$$\alpha_{1/2} = 1 + g_1/\lambda,$$

$$\tilde{u}_5(x; W) = e^{-x/2} x^{1/2} \left[x^{-\mu} \Phi(\alpha_{1/2}, \beta_{1/2}; z) + g_1 \Gamma(\beta_{1/2}) \lambda^{1/2} \Phi(\alpha_{1/2}, \beta_{1/2}; z)\right]_{\alpha_{1/2} \to 1/2},$$

$$\omega_{1/2}(W) = g_1 C + g_1 \left[\psi(\alpha_{1/2}) + \ln(\lambda/k_0)\right] - g_1 - \lambda/2,$$

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

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

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

$$u_5(x; W) = u_{5as}(x) + O(x^2 \ln x),$$

$$u_1(x; W) = \Gamma^{-1}(\alpha_{1/2}) \left[k_0^{-1} \omega_{1/2}(W) u_{1as}(x) + u_{5as}(x)\right] + O(x^2 \ln x),$$

$$u_{1as}(x) = k_0 x, \quad u_{5as}(x) = 1 + g_1 x \ln(k_0/R) + C g_1 x.$$  

(47)
As $x \to \infty$, $\text{Im} \, W > 0$, we have
\[
 u_1(x; W) = G^{-1}(\alpha_{1/2}) \lambda^{-1} \bar{\epsilon}^{1/3} x^{-1/3} e^{i/3} \dot{\Omega}(x^{-1}) \to \infty,
\]
u_1(x; W) = \lambda^{-1} \bar{\epsilon}^{1/3} x^{-1/3} e^{i/3} \dot{\Omega}(x^{-1}) \to 0.

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 equation (4); the same holds for the functions $u_1, v_1$ for $\text{Im} \, W \neq 0$, see section 3.2.

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

As we know from section 3.2, at $g_2 < -1/4$, 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.

To evaluate the asymmetry form $\Delta_{\hat{H}}^\alpha$, we determine the asymptotics of functions $\psi_\alpha$, belonging to $D_{\hat{H}}^\alpha(\mathbb{R}_+)$, at the origin using the representation (23) of the general solution of equation (14) with $W = 0$, where the natural substitutions $\alpha_1 \to \alpha_2$ and $u_2/2\mu \to u_5$ must be made, and estimating the integral terms by means of the Cauchy–Bunyakovsky inequality, which yields
\[
\psi_\alpha(x) = a_1 u_{1\alpha}(x) + a_2 u_{5\alpha}(x) + O(x^{3/2}),
\]
\[
\psi'_\alpha(x) = a_1 u_{1\alpha}'(x) + a_2 u_{5\alpha}'(x) + O(x^{1/2}),
\]
\[
\psi_{5,\alpha}(x) = u_{1\alpha}(k_0 x) \sin \epsilon + u_{5\alpha}(x) \cos \epsilon.
\]

Therefore,
\[
D_{\hat{H}_{\alpha}} = \left\{ \psi : \psi \in D_{\hat{H}}^\alpha(\mathbb{R}_+), \psi \text{ satisfy (48)} \right\}.
\]

To find the Green’s function $G(x, y; W)$ for $\hat{H}_{\alpha}$, we use representation (15) with $a_1 = 0$ for $\psi_\alpha(x)$ belonging to $D_{\hat{H}_{\alpha}} \subset D_{\hat{H}}^\alpha(\mathbb{R}_+)$, boundary conditions (48) and asymptotics (47); then we find that
\[
G(x, y; W) = \Omega^{-1}(W) u_{5,\epsilon}(x; W) u_{5,\epsilon}(y; W) - \frac{1}{k_0} \left[ u_{5,\epsilon}(x; W) u_{5,\epsilon}(y; W), \begin{array}{c} x > y, \\ x < y, \end{array} \right]
\]
where
\[
\Omega(W) = k_0 \left[ k_0 \sin \epsilon - \omega_1/2(W) \cos \epsilon \right] \times \left[ \omega_1/2(W) \sin \epsilon + k_0 \cos \epsilon \right]^{-1},
\]
\[
 u_{5,\epsilon}(x; W) = k_0 \dot{u}_1(x; W) \sin \epsilon + u_5(x; W) \cos \epsilon,
\]
\[
 \dot{u}_5(x; W) = k_0 \dot{u}_1(x; W) \cos \epsilon - u_5(x; W) \sin \epsilon,
\]
\[
 k_0 \Gamma(\alpha_{1/2}) v_1(x; W) = \left[ \omega_1/2(W) \cos \epsilon - k_0 \sin \epsilon \right] \dot{u}_5(x; W) + \left[ \omega_1/2(W) \sin \epsilon + k_0 \cos \epsilon \right] u_5(x; W).
\]

We note that $u_{5,\epsilon}(x; W)$ and $\dot{u}_{5,\epsilon}(x; W)$ are solutions of equation (4) real-entire in $W$, the solution $u_{5,\epsilon}(x; W)$ satisfies boundary conditions (48), and 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 section 3.1, whence it follows that the spectra of $\hat{H}_{\alpha}$ are simple.

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

We first consider the case of $\epsilon = \pi/2$, where we have $u_{5,\pi/2}(x; W) = k_0 u_1(x; W)$ and
\[
\sigma'(E) = (\pi k_0^2)^{-1} \text{Im} \, \Theta(E + i0),
\]
\[
\Theta(W) = g_1 \psi(\alpha_{1/2}) + g_1 \ln(\lambda/k_0) - \lambda/2.
\]

For $E = p^2 \geq 0$, $p \geq 0$, we have
\[
\sigma'(E) = \left| \frac{g_1\epsilon}{2k_0^2} \frac{e^{-\pi\epsilon/2p}}{\sin(\pi\epsilon/2p)} \right| \geq 0.
\]

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$ and $g_1 > 0$, $\alpha_{1/2} = 1 + g_1/2\tau$, the function $\Theta(W)$ 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
\[
\sigma'(E) = \sum_{n \in \mathbb{Z}_+} \frac{4}{k_0^2} \frac{|g_1|}{2+2n} \frac{1}{\sin(\pi\epsilon/2)} \delta(E - E_n),
\]
\[
E_n = - \frac{g_1^2}{(2+2n)^2}, \quad n \in \mathbb{Z}_+.
\]

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

We thus find that for $g_1 > 0$, the spectrum of $\hat{H}_{\pi/2}$ is simple, continuous, and given by $\hat{H}_{\pi/2} \subset \mathbb{R}_+$ and the set of generalized eigenfunctions $U_E(x) = \sqrt{\sigma(E)} u_{5,\pi/2}(x; E), E \geq 0$, forms a complete orthonormalized system in $L^2(\mathbb{R}_+)$. For $g_1 > 0$, the spectrum of $\hat{H}_{\pi/2}$ is simple and given by $\hat{H}_{\pi/2} \subset \mathbb{R}_+ \cup \{ E_n, n \in \mathbb{Z}_+ \}$ and the set of (generalized) eigenfunctions
\[
U_E(x) = \sqrt{\sigma'(E)} u_{5,\pi/2}(x; E), \quad E \geq 0,
\]
\[
U_n(x) = \frac{2}{k_0} \left( \frac{|g_1|}{2+2n} \right)^{3/2} u_{5,\pi/2}(x; E_n), \quad n \in \mathbb{Z}_+.
\]
forms a complete orthonormalized system in $L^2(\mathbb{R}_+)$. We now turn to the case $|\epsilon| < \pi/2$ where we have
\[
\sigma'(E) = (\pi \cos^2 \epsilon)^{-1} \text{Im} \, \omega_3(E + i0)]^{-1},
\]
\[
\omega_3(W) = k_0 \tan \epsilon - \omega_{1/2}(W).
\]

For $g_1 < 0$, $E = p^2 \geq 0$, $p \geq 0$, we have $\lambda = 2p e^{-i\pi/2}$, we find that
\[
\sigma'(E) = \frac{B(E)}{\pi \cos^2 \epsilon [A^2(E) + B^2(E)]},
\]
\[
(49)
\]
where $\omega_5(E) = A(E) - iB(E)$. The function $B(E)$ is explicitly given by

$$B(E) = \frac{\pi}{2} \frac{|g_1| e^{-\pi g_1/2p}}{\sinh(\pi |g_1|/2p)} > 0, \quad \forall p \geq 0. \quad (50)$$

It follows that for $g_1 < 0$, the spectrum of $\hat{H}_{5,\epsilon}$ is purely continuous.

For $g_1 > 0$, $E = p^2 > 0$, $p > 0$, $\lambda = 2p e^{-\pi g_1/2}$, the derivative of the spectral function is also given by equations (49) and (50). But in this case, we have $B(0) = 0$ and the limit $\lim_{\omega \to 0} \omega_5(W)$ has to be carefully examined. For small $W$, we have

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

$$\tan \epsilon_0 = (g_1/\kappa_0) [\ln(g_1/k_0) + C - 1].$$

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

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

which means that the spectrum of the Hamiltonian $\hat{H}_{5,\epsilon}$ 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 $E_n(\epsilon)$ of $\omega_5(E)$ and $\sigma'(E)$ is represented as

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

$$\omega_5(E_n(\epsilon)) = 0, \quad \omega'_5(E_n(\epsilon)) < 0.$$  

For $g_1 > 0$, we have

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

$$\omega_5(E) = \sqrt{|E|} - (g_1/2) \ln |E| + O(1), \quad E \to -\infty,$$

$$\omega_5(0) = k_0(\tan \epsilon - \tan \epsilon_0).$$

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 $E^{(\epsilon)}$ is. It is easy to see that

$$\frac{d}{d\epsilon} E^{(\epsilon)} = -k_0' \omega_5'(E^{(\epsilon)}) \cos^2 \epsilon|^{-1} > 0,$$

so that $E^{(\epsilon)}(\epsilon)$ increases monotonically from $-\infty$ to $0$ when $\epsilon$ changes from $-\pi/2 + 0$ to $\epsilon_0$.

For $g_1 < 0$, we have

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

$$\epsilon = g_1 C - g_1 - k_0 \tan \epsilon.$$

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

$$f(E_n) = \epsilon, \quad f(E) = |g_1|\psi(1/2 - |g_1|/2\tau) + |g_1|\ln(2\tau/k_0) + \tau,$$

we can see that

$$f(E) \xrightarrow{E \to -\infty} \infty, \quad f(E_n \pm 0) = \pm \infty,$$

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

(b) For any fixed $\epsilon$, $E_n(\epsilon) = -g_1^2/(4n^2 + O(n^{-3})$ as $n \to \infty$, asymptotically coinciding with (22).

(c) The point $E = 0$ is an accumulation point of a discrete spectrum for $g_1 < 0$.

Note the relation

$$\lim_{\epsilon \to \pi/2} E_n-1(\epsilon) = \lim_{\epsilon \to -\pi/2} E_n(\epsilon) = \epsilon_n, \quad n \in \mathbb{Z}_n.$$  

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

$$\text{spec } \hat{H}_{5,\epsilon} = \mathbb{R}_+ \cup \{E_n(\epsilon) < 0, \quad n \in (-1) \cup \mathbb{Z}_n\}.$$  

The (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} u_{5,\epsilon}(x; E), \quad E \geq 0,$$

$$u_n(\epsilon) = -\omega_5'(E_n(\epsilon))^{-1/2} u_{5,\epsilon}(x; E_n(\epsilon)), \quad n \in (-1) \cup \mathbb{Z}_n,$$

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

$$\text{spec } \hat{H}_{5,\epsilon} = \mathbb{R}_+ \cup \{E^{(\epsilon)}(\epsilon) \leq 0\}.$$  

For $\epsilon \in (-\pi/2, \epsilon_0]$ the (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} u_{5,\epsilon}(x; E), \quad E \geq 0,$$

$$U(x) = -\omega_5'(E^{(\epsilon)}(\epsilon))^{-1/2} u_{5,\epsilon}(x; E^{(\epsilon)}(\epsilon))$$

form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. For $\epsilon \geq \epsilon_0$, the spectrum has no negative eigenvalues.

We note that the above results (for the spectrum and eigenfunctions) can be extracted from the results in section 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 on the Kratzer potential [6] mentioned in the introduction. This potential corresponds to a particular case of parameters $g_2 > 0$ and $g_1 < 0$. It is shown by the thick line in the graph of figure 1. As was already stated, the Kratzer potential is extensively used to describe the molecular structure and interactions [19]. In such cases, the Kratzer potential appears in the radial part of the Schrödinger equation (2) and has the form

$$V(x) = -2D_x \left(\frac{a}{x} - \frac{1}{2} \frac{a^2}{x^2}\right), \quad (51)$$

where $D_x$ 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 decomposition of molecules. Putting the potential (51) in the radial equation (2) and comparing with the Schrödinger equation (4), we have the following identification:

\[
\begin{align*}
g_1 &= \frac{-4m}{\hbar^2} D_{e1} a, \\
g_2 &= \frac{2m}{\hbar^2} D_{e2} a^2 + l(l + 1).
\end{align*}
\]

We can now calculate the value of \(g_2\) for real diatomic molecules. Using the 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 as for molecules of NO, O\(_2\), I\(_2\) and H\(_2\). Thus, we see that for realistic Kratzer potentials, the corresponding radial equations (2) are always of the form (4) with \(g_2 > 3/4\). Thus, the corresponding radial problem belongs to the first range described in subsection 3.1. In this case, there exists only one s.a. radial Hamiltonian defined on the natural domain (5); functions from this domain have asymptotics (16).

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References

[1] Fues E 1926 Das Eigenschwingungsspektrum zweiatomiger Moleküle in der Undulationsmechanik Ann. Phys., Lpz. 385 367
[2] Scarf S L 1958 Discrete states for singular potential problems Phys. Rev. 109 2170
[3] Flügge S 1994 Practical Quantum Mechanics (Berlin: Springer)
[4] Landau L D and Lifshitz E M 1977 Quantum Mechanics (Oxford: Pergamon)
[5] Bagrov V G and Gitman D M 1990 Exact Solutions of Relativistic Wave Equations (Dordrecht: Kluwer)
[6] Kratzer A 1920 Die ultraroten Rotationsspektren der Halogenwasserstoffe Z. Phys. 3 289
[7] Bayrak O, Boztosun I and Ciftci H 2007 Exact analytical solutions to the Kratzer potential by the asymptotic iteration method Int. J. Quantum Chem. 107 540
[8] Baughan E C 1953 Comments on the thermochemistry of the elements of Groups IVB and IV Q. Rev. 7 103
[9] Mott N F and Massey H S W 1949 Theory of Atomic Collisions (Oxford: Clarendon)
[10] Ballhausen C J and Gajhede M 1990 The tunnel effect and scattering by a negative Kratzer potential Chem. Phys. Lett. 165 449
[11] Eliashевич M A 1962 Atomic and Molecular Spectroscopy (Moscow: State Physical and Mathematical Publishing)
[12] Voronov B L, Gitman D M and Tyutin I V 2007 Constructing quantum observables and self-adjoint extensions of symmetric operators I Russ. Phys. J. 50 1
[13] Voronov B L, Gitman D M and Tyutin I V 2007 Constructing quantum observables and self-adjoint extensions of symmetric operators. II. Differential operators Russ. Phys. J. 50 853
[14] Krein M T 1946 A general method for decomposition of positively defined kernels into elementary products Dokl. Akad. Nauk SSSR 53 3 (in Russian)
[15] Krein M T 1948 On Hermitian operators with guiding functionals Zbirnik Prac’i Instituta Matematiki (AN USR) 10 83 (in Ukrainian)
[16] Naimark M A 1969 Linear Differential Operators (Moscow: Nauka)
[17] Akhiezer N I and Glazman I M 1981 Theory of Linear Operators in Hilbert Space (Boston, MA: Pitman)
[18] Voronov B L, Gitman D M and Tyutin I V 2007 The Dirac Hamiltonian with a superstrong Coulomb field Theor. Math. Phys. 150 34
[19] Voronov B L, Gitman D M and Tyutin I V 2010 Self-adjoint extensions and spectral analysis in the Calogero problem J. Phys. A: Math. Theor. 43 145205
[20] Gitman D M, Tyutin I V, Smirnov A G and Voronov B L 2009 Self-adjoint Schrödinger and Dirac operators with Aharonov–Bohm and magnetic-solenoid fields arXiv:0911.0946 [quant-ph]
[21] Bateman H and Erdelyi A 1953 Higher Transcendental Functions (New York: McGraw-Hill)
[22] Gradshtein I S and Ryzhik N M 1971 Tables of Integrals, Sums, Series and Products (Moscow: Nauka)
[23] Le Roy R J and Bernstein R B 1970 Dissociation energy and long-range potential of diatomic molecules from vibrational spacings of higher levels J. Chem. Phys. 52 3869
[24] Karplus M and Porter R N 1970 Atoms and Molecules (Menlo Park, CA: Benjamin)