The functional–analytic versus the functional–integral approach to quantum Hamiltonians: 
The one–dimensional hydrogen atom

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Abstract

The capabilities of the functional–analytic and of the functional–integral approach for the construction of the Hamiltonian as a self–adjoint operator on Hilbert space are compared in the context of non–relativistic quantum mechanics. Differences are worked out by taking the one–dimensional hydrogen atom as an example, that is, a point mass on the Euclidean line subjected to the inverse–distance potential. This particular choice is made with the intent to clarify a long–lasting discussion about its spectral properties. In fact, for the four–parameter family of possible Hamiltonians the corresponding energy–dependent Green functions are derived in closed form. The multiplicity of Hamiltonians should be kept in mind when modelling certain experimental situations as, for instance, in quantum wires.

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I. INTRODUCTION

This contribution is about a basic aspect of non–relativistic quantum mechanics of a point particle in $d$–dimensional Euclidean space $\mathbb{R}^d$ subjected to a real–valued potential $V(q)$. The first task in characterizing the associated quantum system is to define its Hamiltonian $H$ as a self–adjoint operator acting on the Hilbert space $L^2(\mathbb{R}^d)$ of complex–valued functions which are square–integrable with respect to the Lebesgue measure $d^dq$ in $\mathbb{R}^d$. Principally, there are two different approaches to do so. The functional–analytic approach, see e.g. Refs. [1,2], is concerned with constructing $H$ as a self–adjoint extension of Schrödinger’s formal differential operator $(-1/2)\Delta + V(q)$. Here $\Delta$ denotes the Laplacian in $\mathbb{R}^d$ and units are chosen such that the mass of the particle and Planck’s constant $\hbar$ are equal to unity. In the functional–integral approach, see e.g. Refs. [3–6], the operator $H$ is defined as the (negative) generator of a self–adjoint strongly continuous one–parameter semigroup on $L^2(\mathbb{R}^d)$ which, in turn, is defined as an average of a suitable functional over the paths $x : t \mapsto x(t)$ of a suitable Markov process in $\mathbb{R}^d$ indexed by time $t \geq 0$. Under rather mild assumptions on the potential $V$, both approaches yield naturally the same unique Hamiltonian $H$. For example, this is the case if $V$ is Katō decomposable, that is, if $|V| - V$ and $|V| + V$ are in the Katō and local Katō class over $\mathbb{R}^d$, respectively. The equivalence of both approaches is then concisely expressed by the standard Feynman–Kac formula

$$\langle q_b | \exp \{-tH\} | q_a \rangle = \int_{C(\mathbb{R}^d, q_a)} dW^d[x] \delta^{(d)}(x(t) - q_b) \exp \left\{-\int_0^t dt' V(x(t'))\right\}. \quad (1)$$

Here we have used Dirac’s notation for the integral kernel of the semigroup $\{e^{-tH}\}_{t \geq 0}$. Moreover, $dW^d$ denotes Wiener’s probability measure, which is concentrated on the set $C(\mathbb{R}^d, q_a)$ of continuous paths $x$ in $\mathbb{R}^d$ starting from $q_a \in \mathbb{R}^d$, that is, $x(0) = q_a$. The Dirac delta function accounts for the fact that the paths are conditioned to arrive at $q_b \in \mathbb{R}^d$ at time $t$. In other words, the path average is effectively taken with respect to the Brownian bridge.[7]

As a prominent example we consider the inverse–distance potential $V(q) = -\gamma/|q|$, $\gamma \in \mathbb{R}$. Even though the coupling constant $\gamma$ may take on both signs and this potential coincides only for $d = 3$ with the Newton–Coulomb potential on $\mathbb{R}^d$, we will refer to the associated quantum system as the $d$–dimensional hydrogen atom for all $d \geq 1$. In what follows, an important point is that $-\gamma/|q|$ is Katō decomposable if and only if $d \geq 2$.

The answer to the question, what happens in $d = 1$, will be our main concern here. In fact, a study of the one–dimensional hydrogen atom is of interest for at least two reasons. First, it nicely illustrates subtleties in the functional–analytic and in the functional–integral approach, which are also present in other systems with a sufficiently singular potential. These subtleties, while technical in nature, have important physical consequences. Only if the well–established mathematical techniques for handling them are generally accepted, one may hope for an end of a long–lasting discussion.[8,9] Second, the one–dimensional hydrogen atom is of physical relevance in relation with atoms or excitons in the presence of strong magnetic fields.[10,11,12] or in quantum wires.[13,14] It is also discussed in the semiclassical approximation of quantum dynamics[15] and as a model for an electron near the surface of liquid helium[16].
We will see that the standard functional–analytic approach provides a four–parameter family \( \{ H_B \} \) of self–adjoint extensions of the formal differential operator \((-1/2)d^2/dq^2 - \gamma/|q|\). As is suggested from the singularity of the potential, different \( H_B \) simply correspond to different boundary conditions to be imposed on the wave functions \( \varphi \in L^2(\mathbb{R}) \) at the origin of the real line \( \mathbb{R} \). In contrast, our functional–integral approach, which seeks to keep the RHS of (1) finite by excluding appropriate paths, will yield only one element of the family \( \{ H_B \} \), namely \( H_D \), the one corresponding to a Dirichlet condition at \( q = 0 \). Finally, we take the opportunity to rederive the early closed–form expression for the energy–dependent Green function \( \langle q_b|(H_D - E)^{-1}|q_a\rangle \) by a genuine functional–integral calculation.

In order to avoid a possible confusion, we remark that the divergency of the RHS of (1) for the attractive case \( \gamma > 0 \) of the potential \( V(q) = -\gamma/|q| \) in \( d = 1 \) has nothing to do with a frequently encountered artifact when discretizing the functional integral inappropriately—sometimes referred to as “path collapse”. This artifact occurs even in \( d \geq 2 \).

II. FUNCTIONAL–ANALYTIC APPROACH

In this section we present the main results of the functional–analytic approach to the one–dimensional hydrogen atom. The strategy we are following is the standard one and was used to treat related problems or special cases. The aim is to find a dense domain in the Hilbert space \( L^2(\mathbb{R}) \), on which the formal differential operator \((-1/2)d^2/dq^2 - \gamma/|q|\) is self–adjoint.

As a first step it is often reasonable to define a formally given operator on the space \( \mathcal{C}_0^\infty(\mathbb{R}) \) of arbitrarily often differentiable complex–valued functions with compact support in \( \mathbb{R} \). This is not possible here because of the \( 1/|q| \)–singularity. Therefore we start with the operator \( h := (-1/2)d^2/dq^2 - \gamma/|q| \) on the domain \( \mathcal{D}(h) := \mathcal{C}_0^\infty(\mathbb{R}\setminus\{0\}) \). The operator \( h \) is symmetric, hence closable. The operator closure \( \tilde{h} \) of \( h \) has deficiency indices \( (2,2) \), as can be seen by solving explicitly the corresponding eigenvalue problem in terms of Whittaker’s functions. It follows that there is a four–parameter family \( \{ H_B \} \) of self–adjoint extensions of \( \tilde{h} \) parametrizable by the self–adjoint \( 2 \times 2 \)–matrix \( B = \left( \begin{array}{cc} \rho & \zeta \\ \zeta^* & \lambda \end{array} \right) \), \( \lambda, \rho \in \mathbb{R} \), \( \zeta \in \mathbb{C} \),

\[
H_B := -\frac{1}{2} \frac{d^2}{dq^2} - \frac{\gamma}{|q|} \quad (2)
\]

\[
\mathcal{D}(H_B) := \left\{ \varphi \in L^2(\mathbb{R}) : \varphi, \varphi' \in \mathcal{AC}_{\text{loc}}(\mathbb{R}\setminus\{0\}), \left( \frac{1}{2} \varphi'' - \frac{\gamma}{|q|} \varphi \right) \in L^2(\mathbb{R}), \right. \\
\left. \left( \lim_{q \to 0^+} \left\{ 2\gamma \varphi(q) \ln(|q|) + \varphi'(q) \right\} \right) = B \left( \lim_{q \to 0^+} \varphi(q) \right), \right. \\
\left. \left( \lim_{q \to 0^-} \left\{ 2\gamma \varphi(q) \ln(-|q|) - \varphi'(q) \right\} \right) = B \left( \lim_{q \to 0^-} \varphi(q) \right) \right\}. \quad (3)
\]

Here \( \mathcal{AC}_{\text{loc}}(\Lambda) \) denotes the set of complex–valued functions \( \varphi \) on \( \Lambda \subseteq \mathbb{R} \) which are absolutely continuous on every compact subset of \( \Lambda \), and the first and second derivatives \( \varphi' \) and \( \varphi'' \) of \( \varphi \) are understood to be defined Lebesgue almost everywhere. As limiting cases, we also
allow the entries of the matrix \( B \) to be infinite in order not to have to distinguish too many different cases. For example, one way to arrive at the Dirichlet condition \( \lim_{q \to 0} \varphi(q) = 0 = \lim_{q \to 0} \varphi(q) \) at the origin is by choosing \( \zeta = 0, \lambda = \rho = \infty \). We denote the corresponding Hamiltonian by \( H_D \). In the zero–coupling case \( \gamma = 0 \), each \( H_B \) describes a particle on the real line subjected to a certain point interaction at the origin. \([43] \) In particular, for appropriate \( B \) the \( \delta^- \) and (so–called) \( \delta' \)–interaction emerge.

Remarkably, there is a closed–form expression for the energy–dependent Green function \( \langle q_b | (H_B - E)^{-1} | q_a \rangle \), that is, for the integral kernel of the resolvent of \( H_B \). Since this expression involves the Green function of \( H_D \), we first state

\[
\langle q_b | (H_D - E)^{-1} | q_a \rangle = \Theta(q_b q_a) \frac{\Gamma(1 - \gamma/\sqrt{-2E})}{\sqrt{-2E}} \\
\times \left[ \Theta(|q_b| - |q_a|) W_{\gamma/\sqrt{-2E},1/2}(\sqrt{-8E}|q_b|) M_{\gamma/\sqrt{-2E},1/2}(\sqrt{-8E}|q_a|) \\
+ (q_b \leftrightarrow q_a) \right].
\]

(4)

Here \( \Theta \) denotes Heaviside’s unit–step function, \( \Gamma \) denotes Euler’s gamma function and \( M_{\mu,\tau} \) and \( W_{\mu,\tau} \) denote Whittaker’s functions. \([3] \) For \( q_a, q_b \geq 0 \), Eq. (4) is just the Green function of the hydrogen atom on the positive half–line with a Dirichlet condition at the origin. Being the \( s \)–wave part of the Green function of the three–dimensional hydrogen atom (apart from a factor \( 4\pi q_b q_a \)), it appeared for the first time in the early work of Meixner \([3] \) as a by–product. The second part of the next section will be devoted to a genuine functional–integral derivation of (4).

For completeness and convenience of the reader we recall for the attractive case \( \gamma > 0 \) the twofold degenerate discrete eigenvalues \( E^{(D)}_n \) and give an orthonormal basis \( \{ \varphi^{(D)}_{n,1}, \varphi^{(D)}_{n,2} \} \) of the corresponding two–dimensional eigenspaces of \( H_D \) as obtained from the poles and corresponding residues of (4)

\[
E^{(D)}_n = -\frac{\gamma^2}{2n^2}, \quad n = 1, 2, 3, \ldots,
\]

(5)

\[
\varphi^{(D)}_{n,k}(q) = \Theta\left( (-1)^k q \right) \frac{2\gamma^{3/2}}{n^{5/2}} |q| e^{-|q|^{\gamma/n}} L^{(1)}_{n-1}(2 |q| \gamma/n), \quad k = 1, 2.
\]

(6)

Here \( L^{(a)}_n \) denotes a (generalized) Laguerre polynomial \([43] \)

Green functions of different self–adjoint extensions of a closed symmetric operator are related via a Krein formula. \([4] \) Its particularization to the case of the one–dimensional hydrogen atom gives

\[
\langle q_b | (H_B - E)^{-1} | q_a \rangle = \langle q_b | (H_D - E)^{-1} | q_a \rangle + 2 \left( \Gamma(1 - \gamma/\sqrt{-2E}) \right)^2 \\
\times W_{\gamma/\sqrt{-2E},1/2}(\sqrt{-8E}|q_b|) W_{\gamma/\sqrt{-2E},1/2}(\sqrt{-8E}|q_a|) \\
\times (\Theta(q_b), \Theta(-q_b)) \left( B - \varepsilon_{\gamma}(E)I \right)^{-1} \left( \begin{array}{c} \Theta(q_a) \\ \Theta(-q_a) \end{array} \right),
\]

(7)
where
\[ \varepsilon_\gamma(E) := 2\gamma \left[ \ln(|\gamma|/\sqrt{-8E}) - \psi(1 - \gamma/\sqrt{-2E}) + 2\psi(1) \right] - \sqrt{-2E} \] (8)
and \( \psi(z) := d \ln \Gamma(z)/dz \) is the logarithmic derivative of Euler’s gamma function.

Since the deficiency indices of \( \tilde{h} \) are finite, all self–adjoint extensions \( H_B \) possess the same essential spectrum \( \sigma_{\text{ess}}(H_B) = [0, \infty[ \). For the same reason and due to the fact that \( H_D \) is bounded below, see e.g. Eq. (1) above, one concludes that they are all bounded below. The discrete spectrum of \( H_B \) is obtained from the poles of (7) and consists of those \( E \in ] - \infty, 0[ \) for which \( \varepsilon_\gamma(E) \) is an eigenvalue of
\[ 2\varepsilon_\gamma(E) = \lambda + \rho \pm \sqrt{(\lambda - \rho)^2 + 4|\zeta|^2}. \] (9)
A plot of \( \varepsilon_\gamma/\gamma \) for \( E < 0 \) as a function of \( \gamma/\sqrt{-2E} \) is given in Figure 1. It turns out that the discrete spectrum is twofold degenerate, if \( \zeta = 0 \) and \( \lambda = \rho \). Not unexpectedly, for \( \gamma > 0 \) there are infinitely many discrete eigenvalues irrespective of the choice of \( B \). Even for \( \gamma < 0 \) there may be one or two negative discrete eigenvalue(s). For a given coupling constant \( \gamma \in \mathbb{R} \) one can choose the matrix \( B \) and thus the boundary condition in such a way that the ground–state energy of \( H_B \) is arbitrarily negative.

An interesting quantity to look at is the probability current density \( j_\varphi(q) := \text{Im}\{\varphi^*(q)\varphi'(q)\} \) for \( \varphi \in \mathcal{D}(H_B) \). Due to self–adjointness it is continuous in \( q \) for all \( q \in \mathbb{R} \), even at the origin, where it is given by
\[ j_\varphi(0) = \text{Im}\{\zeta \lim_{q\downarrow 0} \varphi^*(q)\varphi(-q)\}. \] (10)
In consequence, the choice \( \zeta = 0 \) implies \( j_\varphi(0) = 0 \) for all \( \varphi \in \mathcal{D}(H_B) \), which means that the real line is effectively split into its negative and positive half by the \( 1/|q| \)–singularity. It is only the resulting two–parameter subfamily that can be obtained as the orthogonal sum of two Hamiltonians each of which is defined separately on the Hilbert space corresponding to one of the half–lines. Thorough discussions of the one–parameter family of Hamiltonians associated with the one–dimensional hydrogen atom on the half–line have been given earlier, see Refs. [39–41].

III. FUNCTIONAL–INTEGRAL APPROACH

As already mentioned in the Introduction, the Wiener integral on the rhs of (1) for the \( d \)–dimensional hydrogen atom is well–defined and finite for all \( d \geq 2 \). By now, also the explicit evaluation of the Laplace transform of such functional integrals is well–established. The one–dimensional case was explicitly considered in Ref. [55] by formally setting \( d = 1 \) in the final result of such an evaluation without any justification. The trouble with this procedure is that one does not know \textit{a priori} to which physical problem it yields the solution. Instead, as a first step it is necessary to discuss the question of how the hydrogen atom can be reasonably defined in one dimension from the point of view of functional integration.

To begin with, we clarify for which paths \( x \) of the one–dimensional Wiener process with starting point \( q_0 \in \mathbb{R} \) the integral \( \int_0^t dt'/|x(t')| \) is finite. Due to continuity, one has the following inclusion between path sets
\[ N_t(\mathbb{R}, q_a) := \left\{ x \in C(\mathbb{R}, q_a) : x(t') \neq 0 \text{ for all } t' \in [0, t] \right\} \]

\[ \subseteq \left\{ x \in C(\mathbb{R}, q_a) : \int_0^t \frac{dt'}{|x(t')|} < \infty \right\}. \quad (11) \]

Introducing the local time\[ \text{ of } x \text{ at } q, \] which is formally given by \[ L_{t,q}[x] = \int_0^t \delta(1)(x(t') - q), \]

one can write

\[ \int_0^t \frac{dt'}{|x(t')|} = \int_\mathbb{R} \frac{dq}{|q|} L_{t,q}[x]. \quad (12) \]

Hence we deduce a further inclusion

\[ \left\{ x \in C(\mathbb{R}, q_a) : \int_0^t \frac{dt'}{|x(t')|} < \infty \right\} \subseteq \left\{ x \in C(\mathbb{R}, q_a) : L_{t,0}[x] = 0 \right\}. \quad (13) \]

Accordig to Ref. [62], the set \[ N_t(\mathbb{R}, q_a) \] equals almost surely (a.s.) the set on the RHS of (13). Therefore one infers the a.s.–equality

\[ N_t(\mathbb{R}, q_a) = \left\{ x \in C(\mathbb{R}, q_a) : \int_0^t \frac{dt'}{|x(t')|} < \infty \right\}, \quad (14) \]

which is a special case of the Theorem on p. 785 in Ref. [3].

After this prelude the following definition for the functional integral of the one–
dimensional hydrogen atom will suggest itself

\[ \int_{N_t(\mathbb{R}, q_a)} dW^1[x] \delta^{(1)}(x(t) - q_b) \exp \left\{ \int_0^t \frac{\gamma}{|x(t')|} dt' \right\}. \quad (15) \]

Five remarks are in order.

(i) Cor. 6.3.10 in Ref. [63] implies that the restriction of the Wiener measure to \[ N_t(\mathbb{R}, q_a) \]
yields again a Markovian path measure which is invariant under time reversal, namely
the measure corresponding to the Wiener process on \[ \mathbb{R} \] killed at the origin. Using this
fact and

\[ \lim_{t \downarrow 0} \sup_{q \in \mathbb{R}} \int_{N_t(\mathbb{R}, q)} dW^1[x] \int_0^t \frac{dt'}{|x(t')|} = 0, \quad (16) \]

it follows from the appropriate versions of Nakao’s inequality\[ [64] \] and Khas’minskii’s
lemma\[ [65] \] that the functional integral (15) exists.
(ii) Similar to the proof of Thm. B.1.1 in Ref. 7, the Cauchy–Schwarz inequality together with (i) imply that (13) is the integral kernel of a self–adjoint semigroup on $L^2(\mathbb{R})$. This semigroup is strongly continuous, as can be seen by adapting the proof of Thm. 3.1 in Ref. 66, see also Prop. 3.2 in Ref. 5.

(iii) The generator of the semigroup defined by (13) is the Dirichlet Hamiltonian $H_D$ of Sec. II. This follows from the Feynman–Kac formula of Thm. 6.3.12 in Ref. 63, and the fact that $1/|q|$ is operator bounded with respect to the Dirichlet Laplacian with relative bound zero.

(iv) Restricting the paths to the set $N_t(\mathbb{R},q_a)$ is necessary for (15) to exist in the attractive case $\gamma > 0$.

(v) In the repulsive case $\gamma < 0$ the restriction does not have any effects, if one adopts the convention $e^{-\infty} := 0$. This illustrates the fact that the existence of the unrestricted Wiener integral on the rhs of (1) does not necessarily imply that the functional–analytic approach leads to a unique Hamiltonian.

In the second part of this section we will sketch how to obtain the Green function of $H_D$ by computing

$$
\langle q_b | (H_D - E)^{-1} | q_a \rangle = \int_0^\infty dt \ e^{Et} \langle q_b | e^{-tH_D} | q_a \rangle = \int_0^\infty dt \ e^{Et} \int_{N_t(\mathbb{R},q_a)} dW^{(1)}[x] \delta^{(1)}(x(t) - q_b) \exp \left\{ \int_0^t dt' \gamma \frac{|x(t')|}{x(t')} \right\}
$$

for complex energies $E$ with a real part smaller than the infimum of the spectrum of $H_D$. Thereby we follow ideas presented in Refs. 48–60,68–70, where a more recent technique in functional integration, namely path–dependent time transformations, has been developed for quantum–mechanical applications. It is only with the help of this technique that a number of potential systems have been treated exactly in the framework of functional integration. We are going to present only its main ideas, but all steps which are needed for the calculation of (17) will be explained. For a detailed and fairly pedagogical approach to path–dependent time transformations, the reader may consult Refs. 56,58–60,68.

In what follows it will be convenient to introduce the Bessel process with index $1/2$, which is a continuous Markov process taking on values in the positive half–line $\mathbb{R}_+$. It is characterized by the transition density

$$
b_t^{(1/2)}(q',q) := \frac{q'}{q} (2\pi t)^{-1/2} \left( \exp \left\{ -\frac{(q' - q)^2}{2t} \right\} - \exp \left\{ -\frac{(q' + q)^2}{2t} \right\} \right) , \quad q',q \in \mathbb{R}_+ .
$$

Hence, $\Theta(qq')(q'/q)b_t^{(1/2)}(|q'|,|q|) , q',q \in \mathbb{R}$, is the (non–normalized) transition density of the Wiener process on $\mathbb{R}$ killed at the origin and the second line in (17) can be rewritten as $\Theta(q_b q_a)q_a/q_b$ times.

\[ \text{7} \]
where

\[ \int_0^\infty dt \ e^{Et} \int_{C(\mathbb{R}_+, |q_b|)} dB_{1/2}[x] \delta^{(1)}(t - |q_b|) \exp \left\{ \frac{t}{\gamma} \frac{\gamma(t) - |q_b|}{x(t')} \right\} . \]  

(19)

Here \( dB_{1/2} \) denotes the probability measure associated with the Bessel process with index 1/2.

The key for the calculation of (19) is the equality of measures

\[ dB_{1/2} = S(dW^4). \]  

(20)

It states that the measure of the Bessel process with index 1/2 arises as the image of the four–dimensional Wiener measure under the transformation \( S \), which maps the set \( C(\mathbb{R}^4, r_a) \) of paths \( y \) onto the set \( C(\mathbb{R}_+, |q_a|) \) of paths \( x \) according to

\[ x(t) = (Sy)(t) := [y(s_y(t))]^2, \quad r_a^2 := |q_a|. \]  

(21)

Here \( s_y(t) \) is defined to be the inverse mapping of the path–dependent time

\[ t_y(s) := \int_0^s ds' 4(y(s'))^2, \]  

(22)

that is, \( t_y(s_y(t)) = t \). Taking (20) for granted, for the time being, we can rewrite (13) in terms of the paths \( y \)

\[ (19) = 4|q_b| \int_0^\infty ds \ e^{4\gamma s} \int_{C(\mathbb{R}_+, r_a)} dW^4[y] \delta^{(1)}((y(s))^2 - |q_b|) \exp \left\{ 4E \int_0^s ds' (y(s'))^2 \right\} . \]  

(23)

In doing so, we have performed the change–of–variables \( t' \mapsto s' := s_y(t') \), which is possible since \( t_y(s) \) is \( dW^4 \)-a.s. strictly increasing in \( s \), and we have used \( t_y(\infty) = \infty \). \( dW^4 \)-a.s.

In order to calculate (23) we remark that

\[ \delta^{(1)}((y(s))^2 - |q_b|) = \frac{|q_b|}{2} \int d^3\Omega_{r_b} \delta^{(4)}(y(s) - r_b), \]  

(24)

where \( \int d^3\Omega_{r_b} (\bullet) \) stands for the integration with respect to the usual rotational invariant measure on the unit sphere in \( \mathbb{R}^4 \) over the three angles of \( r_b \in \mathbb{R}^4 \) in spherical co–ordinates. Using the well–known explicit expression for the integral kernel of the semigroup generated by the four–dimensional isotropic harmonic oscillator with spring constant \( \omega^2 := -8E \), the RHS of (23) can be cast into the form

\[ \frac{q_b^2}{2} \left( \frac{\omega}{\pi} \right)^2 \int_0^\infty ds \ \exp \left\{ \frac{4\gamma s}{\sinh(\omega s)} \right\} \exp \left\{ -\frac{\omega}{2} (|q_b| + |q_a|) \coth(\omega s) \right\} \]

\[ \times \int d^3\Omega_{r_b} \exp \left\{ \frac{\omega}{\sinh(\omega s)} r_b \cdot r_a \right\} . \]  

(25)
Applying the formula

\[
\int d^3\Omega_{r_b} \exp\left\{ \frac{(2\pi)^2}{z|r_b||r_a|} \right\} = I_1(z|r_b||r_a|)
\]  

(26)

\( z \in \mathbb{R}, \ I_\nu \) denotes the modified Bessel function of the first kind with index \( \nu \) and performing the Laplace transformation, the expression (19) is eventually seen to be identical to

\[
(2|q_b/\omega|q_a|) \Gamma(1 - 2\gamma/\omega) \left( \Theta(|q_b| - |q_a|) W_{2\gamma/\omega,1/2}(\omega|q_b|) M_{2\gamma/\omega,1/2}(\omega|q_a|) + (q_b \leftrightarrow q_a) \right).
\]  

(27)

Since the Green function is analytic on the complement of the spectrum of \( H_D \), the desired result (4) follows from (27), provided that (20) holds.

Following Ref. 68, the validity of the equality of measures (20) with \( S \) as in (21) is implied by the equality

\[
\int_0^\infty dt \ e^{Et} \int_{C(\mathbb{R},|q_a|)} dB_{1/2}[x] \delta^{(1)}(x(t) - |q_b|)
\]

\[
= 4|q_b| \int_0^\infty ds \int_{C(\mathbb{R}^4,r_a)} dW^4[y] \delta^{(1)}(\{y(s)\}^2 - |q_b|) \exp\left\{ 4E \int_0^s ds' (y(s'))^2 \right\},
\]  

(28)

which is nothing but the free–particle version \( \gamma = 0 \) of (23).

To verify (28) we reduce (27) for the case \( \gamma = 0 \) with the help of Ref. 78 to

\[
\frac{|q_b/q_a|}{\sqrt{-2E}} \left( \exp\left\{ \sqrt{-2E} \ |q_b| + |q_a| \right\} - \exp\left\{ \sqrt{-2E} \ |q_b| - |q_a| \right\} \right),
\]  

(29)

which is indeed the Laplace transform of the transition density \( b_t^{(1/2)}(|q_b|, |q_a|) \).

Within the theory of stochastic differential equations there are other ways to prove the equality of measures (20). In essence, they rely on Itô’s formula and on a theorem due to Dambis, Dubins and Schwarz.

To summarize, the path–dependent time transformation (21) relates the energy–dependent Green function of the one–dimensional hydrogen atom, which is the Laplace transform of the non–Gaussian functional integral (14), to the Green function of a four–dimensional harmonic oscillator (23), that is, to the Laplace transform of a Gaussian functional integral, which is explicitly known. The rôle of the spring constant is thereby played by the energy of the hydrogen atom and the rôle of the energy of the harmonic oscillator is played by the coupling constant \( \gamma \).

A path–dependent time transformation similar to (21) was used in previous functional–integral calculations for the radial Green function of the hydrogen atom in two or more dimensions. Further aspects of the relation between the hydrogen atom and the harmonic oscillator in the framework of the stationary Schrödinger equation may be found, e.g., in Refs. 31, 32.
IV. DISCUSSION

Clearly, mathematics alone cannot tell which particular element of the four-parameter family of Hamiltonians \( \{ H_B \} \) should be chosen to model a given experimental situation. Instead, additional physical information is necessary. In this context it is useful to know that, for example, the sequence of Hamiltonians corresponding to the cut-off potentials \(-\gamma/(|q|+a)\) converges in uniform resolvent sense to the Dirichlet Hamiltonian \( H_D \) as \( a \downarrow 0 \).

Another fact which makes \( H_D \) stand out is that the domains of all other self-adjoint extensions contain wave functions for which the expectation values of both the kinetic and the potential energy are infinite—though their sum, the total energy, is always finite. Among the domains \( \mathcal{D}(H_B) \) it is only \( \mathcal{D}(H_D) \) on which one can define the kinetic energy \(-\frac{1}{2}\frac{d^2}{dq^2}\) as a self-adjoint operator. In this light, it is no surprise that the functional–integral approach in Sec. III is only able to yield \( H_D \). Indeed, there it was required to average the Feynman–Kac functional \( \exp\{-\int_0^t dt' V(x(t'))\} \) with respect to a path measure generated by the kinetic energy. By abandoning this requirement, it is shown in Refs. 3,83,84 that the functional–integral approach can also provide self-adjoint extensions other than the Dirichlet Hamiltonian. The price one has to pay is a suitable regularization of the potential near the singularity and a subsequent limit. For an interesting construction of a family of path measures corresponding to \( \{ H_B \} \) in the zero-coupling case, see Ref. 6.

So far, there is no systematic functional–integral analogue of the calculus of deficiency indices in the functional–analytic approach. To develop such an analogue would be an interesting programme for future research.

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REFERENCES

1. N. I. Akhiezer and I. M. Glazman, *Theory of linear operators in Hilbert space*, vol. II (Pitman, Boston, 1981).
2. M. Reed and B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self–Adjointness* (Academic, New York, 1975).
3. H. Ezawa, J. R. Klauder and L. A. Shepp, “Vestigial effects of singular potentials in diffusion theory and quantum mechanics,” J. Math. Phys. 16, 783–799 (1975).
4. H. P. McKean, “$−\Delta$ plus a bad potential,” J. Math. Phys. 18, 1277–1279 (1977).
5. R. Carmona, “Regularity Properties of Schrödinger and Dirichlet Semigroups,” J. Funct. Anal. 33, 259–296 (1979).
6. M. Carreau, E. Farhi and S. Gutmann, “Functional integral for a free particle in a box,” Phys. Rev. D 42, 1194–1202 (1990).
7. B. Simon, “Schrödinger Semigroups,” Bull. Amer. Math. Soc. (N.S.) 3, 447–526 (1982); Erratum: *ibid.* 11, 42 (1984).
8. B. Simon, *Functional Integration and Quantum Physics* (Academic, New York, 1979).
9. G. Roepstorff, *Path Integral Approach to Quantum Physics: An Introduction* (Springer, Berlin, 1994).
10. P. Protter, *Stochastic integration and differential equations: a new approach*, 2nd corrected printing (Springer, Berlin, 1992).
11. R. Loudon, “One–Dimensional Hydrogen Atom,” Am. J. Phys. 27, 649–655 (1959).
12. M. Andrews, “Ground State of the One–Dimensional Hydrogen Atom,” Am. J. Phys. 34, 1194–1195 (1966).
13. L. K. Haines and D. Roberts, “One–Dimensional Hydrogen Atom,” Am. J. Phys. 37, 1145–1154 (1969).
14. M. Andrews, “Singular potentials in one dimension,” Am. J. Phys. 44, 1064–1066 (1976).
15. J. F. Gomes and A. H. Zimerman, “One–dimensional hydrogen atom,” Am. J. Phys. 48, 579–580 (1980).
16. M. Andrews, “Comment on the ‘One–dimensional hydrogen atom’,” Am. J. Phys. 49, 1074 (1981).
17. R. E. Moss, “The hydrogen atom in one dimension,” Am. J. Phys. 55, 397–401 (1987).
18. L. S. Davtyan, G. S. Pogosyan, A. N. Sissakian and V. M. Ter–Antonyan, “On the hidden symmetry of a one–dimensional hydrogen atom,” J. Phys. A 20, 2765–2772 (1987).
19. C. L. Hammer and T. A. Weber, “Comments on the one–dimensional hydrogen atom [Am. J. Phys. 27, 649 (1959); Am. J. Phys. 37, 1145 (1969); Am. J. Phys. 44, 1064 (1976)],” Am. J. Phys. 56, 281–282 (1988).
20. M. Andrews, “The one–dimensional hydrogen atom,” Am. J. Phys. 56, 776 (1988).
21. H. N. Núñez Yépez, C. A. Vargas and A. L. Salas Brito, “Superselection rule in the one–dimensional hydrogen atom,” J. Phys. A 21, L651–L653 (1988).
22. L. J. Boya, M. Kmiecik and A. Bohm, “Hydrogen atom in one dimension,” Phys. Rev. A 37, 3567–3569 (1988); Erratum: *ibid.* 40, 6729 (1989).
23. H. N. Núñez Yépez, C. A. Vargas and A. L. Salas Brito, “Comment on ‘Hydrogen atom in one dimension’,” Phys. Rev. A 39, 4306–4307 (1989).
24. U. Oseguera and M. de Llano, “Two singular potentials: The space–splitting effect,” J. Math. Phys. 34, 4575–4589 (1993).
25 M. Moshinsky, “Penetrability of a one–dimensional Coulomb potential,” J. Phys. A 26, 2445–2450 (1993).
26 R. G. Newton, “Comment on ‘Penetrability of a one–dimensional Coulomb potential’ by M Moshinsky,” J. Phys. A 27, 4717–4718 (1994).
27 M. Moshinsky, “Response to “Comment on ‘Penetrability of a one–dimensional Coulomb potential’ ” by Roger G Newton,” J. Phys. A 27, 4719–4721 (1994).
28 R. J. Elliott and R. Loudon, “Theory of the absorption edge in semiconductors in a high magnetic field,” J. Phys. Chem. Solids 15, 196–207 (1960).
29 H. Ruder, G. Wunner, H. Herold and F. Geyer, Atoms in strong magnetic fields (Springer, Berlin, 1994).
30 J. Lee and H. N. Spector, “Hydrogenic impurity states in a quantum well wire,” J. Vac. Sci. Technol. B 2, 16–20 (1984).
31 G. W. Bryant, “Hydrogenic impurity states in quantum–well wires,” Phys. Rev. B 29, 6632–6639 (1984).
32 L. Bányai, I. Galbraith, C. Ell and H. Haug, “Excitons and biexcitons in semiconductor quantum wires,” Phys. Rev. B 36, 6099–6104 (1987).
33 S. Abe, “Exciton versus Interband Absorption in Peierls Insulators,” J. Phys. Soc. Jpn. 58, 62–65 (1989).
34 T. Ogawa and T. Takagahara, “Optical absorption and Sommerfeld factors of one–dimensional semiconductors: An exact treatment of excitonic effects,” Phys. Rev. B 44, 8138–8156 (1991).
35 I. M. Suarez Barnes, M. Nauenberg, M. Nockleby and S. Tomsovic, “Semiclassical Theory of Quantum Propagation: The Coulomb Potential,” Phys. Rev. Lett. 71, 1961–1964 (1993).
36 G. F. Saville and J. M. Goodkind, “Computation of tunneling rates in time–dependent electric fields: Electrons on the surface of liquid helium, a one–dimensional hydrogen atom,” Phys. Rev. A 50, 2059–2067 (1994).
37 J. Meixner, “Die Greensche Funktion des wellenmechanischen Keplerproblems,” Math. Z. 36, 677–707 (1933).
38 H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics, 2nd edition (World Scientific, Singapore, 1995).
39 F. Rellich, “Die zulässigen Randbedingungen bei den singulären Eigenwertproblemen der mathematischen Physik,” Math. Z. 49, 706–723 (1943/44).
40 W. Bulla and F. Gesztesy, “Deficiency indices and singular boundary conditions,” J. Math. Phys. 26, 2520–2528 (1985).
41 S. Albeverio, F. Gesztesy, R. Høegh–Krohn and H. Holden, Solvable Models in Quantum Mechanics (Springer, New York, 1988).
42 S. Albeverio, Z. Brežniak and L. Dąbrowski, “Time–dependent propagator with point interaction,” J. Phys. A 27, 4933–4943 (1994).
43 I. S. Gradshteyn and I. M. Ryzhik Table of Integrals, Series, and Products, corrected and enlarged edition (Academic, San Diego, 1980).
44 §127 in Ref. I.
45 App. A in Ref. I.
46 Thm. 1 on p. 365 in Ref. I.
47 Prop. on p. 179 in Ref. I.
48 I. H. Duru and H. Kleinert, “Solution of the Path Integral for the H–Atom,” Phys. Lett.
49 Ph. Blanchard and M. Sirugue, “Treatment of some singular potentials by change of variables in Wiener integrals,” J. Math. Phys. 22, 1372–1376 (1981).

50 R. Ho and A. Inomata, “Exact–Path–Integral Treatment of the Hydrogen Atom,” Phys. Rev. Lett. 48, 231–234 (1982).

51 A. Inomata, “Alternative Exact–Path–Integral Treatment of the Hydrogen Atom,” Phys. Lett. A 101, 253–257 (1984).

52 F. Steiner, “Exact Path Integral Treatment of the Hydrogen Atom,” Phys. Lett. A 106, 363–367 (1984).

53 N. K. Pak and I. Sökmen, “General new–time formalism in the path integral,” Phys. Rev. A 30, 1629-1635 (1984).

54 F. Steiner, “Path Integrals in Polar Co–ordinates from eV to GeV,” in Path Integrals from meV to MeV, pp. 335–359, edited by M. C. Gutzwiller, A. Inomata, J. R. Klauder and L. Streit (World Scientific, Singapore, 1986).

55 L. Chetouani and T. F. Hammann, “Coulomb Green’s functions, in an n–dimensional Euclidean Space,” J. Math. Phys. 27, 2944–2948 (1986).

56 A. Young and C. DeWitt–Morette, “Time Substitution in Stochastic Processes as a Tool in Path Integration,” Ann. Phys. (NY) 169, 140–166 (1986).

57 H. Kleinert, “How to do the time sliced path integral of the H atom,” Phys. Lett. A 120, 361–366 (1987).

58 D. P. L. Castrigiano and F. Stärk, “New aspects of the path integrational treatment of the Coulomb potential,” J. Math. Phys. 30, 2785–2788 (1989).

59 D. P. L. Castrigiano and F. Stärk, “Intrinsic Clock as a Tool for Path Integration: An Example” in White Noise Analysis, Mathematics and Applications, pp. 49-65, edited by T. Hida et al (World Scientific, Singapore, 1990).

60 D. P. L. Castrigiano and F. Stärk, “General Aspects of the Space and Time Transformations for the Coulomb Propagator” in Quantum Probability VI, pp. 245–258, edited by L. Accardi (World Scientific, Singapore, 1991).

61 D. Revuz and M. Yor, Brownian Motion and Continuous Martingales, 2nd edition (Springer, Berlin, 1994).

62 Remark 1 on p. 208 in Ref. [51].

63 O. Bratteli and D. W. Robinson, Operator Algebras and Quantum Statistical Mechanics, vol. II (Springer, New York, 1981).

64 S. Nakao, “On the spectral distribution of the Schrödinger operator with random potential,” Japan. J. Math. 3, 111–139 (1977), Remark 3.2.

65 M. Aizenman and B. Simon, “Brownian Motion and Harnack Inequality for Schrödinger Operators,” Commun. Pure Appl. Math. 35, 209–273 (1982).

66 K. Broderix, D. Hundertmark and H. Leschke, “Continuity properties of Schrödinger semigroups with magnetic fields,” Preprint of the Universities Göttingen, Bochum and Erlangen–Nürnberg.

67 F. Gesztesy, “On the one–dimensional Coulomb Hamiltonian,” J. Phys. A 13, 867–875 (1980).

68 W. Fischer, H. Leschke and P. Müller, “Changing dimension and time: two well–founded and practical techniques for path integration in quantum physics,” J. Phys. A 25, 3835–3853 (1992).
W. Fischer H. Leschke and P. Müller, “Path integration in quantum physics by changing the drift of the underlying diffusion process: Applications of Legendre processes,” Ann. Phys. (NY) 227, 206–221 (1993).

W. Fischer H. Leschke and P. Müller, “Path integration in quantum mechanics by changing drift and time of the underlying diffusion process,” in Path Integrals from meV to MeV: Tutzing ’92, pp. 259–267, edited by H. Grabert, A. Inomata, L. Schulman and U. Weiss (World Scientific, Singapore, 1993).

K. Itô and H. P. McKean, Jr., Diffusion Processes and their Sample Paths, 2nd corrected printing (Springer, Berlin, 1974).

Confer also Eq. (17) in Ref. 68.

(2.7) Prop. in Ch. V in Ref. 61.

Thm. 7.12 in Ref. 8

Formula 8.431.1 in Ref. 43; for hyperspherical polar co–ordinates in four dimensions, see e.g. A. Erdélyi (Ed.), Higher Transcendental Functions, vol. 2 (McGraw–Hill, New York, 1953), formulae 11.1.1 (7) – (10).

Formula 6.669.4 in Ref. 43 together with the change–of–variables \( \sinh(\omega s) = \frac{1}{\sinh x} \).

M. Reed and B. Simon, Methods of Modern Mathematical Physics I: Functional Analysis, Revised and Enlarged Edition (Academic, New York, 1980); Thm. VIII.2.

Formulae 9.235.1, 9.235.2, 8.467 and 8.469.3 in Ref. 43.

Formulae 3.471.9 and 8.469.3 in Ref. 43.

(3.3) Thm. in Ch. IV, (1.6) Thm. and (1.9) Thm. in Ch. V in Ref. 61.

G. Junker, “Remarks on the local time rescaling in path integration,” J. Phys. A 23, L881–L884 (1990).

D. S. Bateman, C. Boyd and B. Dutta–Roy, “The mapping of the Coulomb problem into the oscillator,” Am. J. Phys. 60, 833–836 (1992).

E. Farhi and S. Gutmann, “The Functional Integral on the Half–Line,” Int. J. Mod. Phys. A 5, 3029–3051 (1990).

M. Carreau, E. Farhi, S. Gutmann and P. F. Mende, “The Functional Integral for Quantum Systems with Hamiltonians Unbounded from Below,” Ann. Phys. (NY) 204, 186–207 (1990).
FIG. 1. Plot of $\frac{\varepsilon_\gamma}{\gamma}$ for $E < 0$ as a function of $\gamma/\sqrt{-2E}$, where $\varepsilon_\gamma$ is defined in Eq. (8). The value of $\frac{\varepsilon_\gamma}{\gamma}$ approaches $4\psi(1) - 2\ln 2 = -3.695\ldots$ as $\gamma/\sqrt{-2E} \to -\infty$. 