

Factor Ordering and Path Integral Measure for Quantum Gravity in (1+1) Dimensions

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Abstract. We develop a mathematically rigorous path integral representation of the time evolution operator for a model of (1+1) quantum gravity that incorporates factor ordering ambiguity. In obtaining a suitable integral kernel for the time-evolution operator, one requires that the corresponding Hamiltonian is self-adjoint; this issue is subtle for a particular category of factor orderings. We identify and parametrize a complete set of self-adjoint extensions and provide a canonical description of these extensions in terms of boundary conditions. Moreover, we use Trotter-type product formulae to construct path-integral representations of time evolution.

Key words: factor ordering in quantum gravity; path integrals in quantum gravity; singularity avoidance in quantum gravity; quantization on a half-line

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1 Introduction

In general relativity, the configuration space for the gravitational field presents two formidable challenges to quantization: first, it is curved, and second, it has a boundary. In terms of Arnowitt–Deser–Misner (ADM) metric variables, the curvature of the configuration space of 3-metrics h_{ab} on a spacelike slice is evident in the DeWitt supermetric

$$G_{abcd} = \frac{1}{2\sqrt{h}}(h_{ac}h_{bd} + h_{ad}h_{bc} - h_{ab}h_{cd}), \quad (1.1)$$

which appears in the kinetic term of the Hamiltonian constraint

$$\mathcal{H} = G_{abcd}\pi^{ab}\pi^{cd} - \sqrt{h}({}^{(3)}R - 2\Lambda) \quad (1.2)$$

generating time-reparametrization invariance. Here $\pi^{ab} = \sqrt{h}(h^{ab}K - K^{ab})$ is the momentum canonically conjugate to h_{ab} , defined in terms of the extrinsic curvature K_{ab} of the spacelike slice. The potential term of the Hamiltonian constraint (1.2) involves the scalar curvature ${}^{(3)}R$ of h_{ab} and a cosmological constant Λ . The difficulty for quantization engendered by the DeWitt supermetric lies in the ambiguity as to how noncommuting operators $\hat{\pi}^{ab}$ and \hat{h}_{ab} are to be ordered in the canonically quantized Hamiltonian constraint, i.e., the Wheeler–DeWitt equation $\hat{\mathcal{H}}\Psi = 0$.

The second problem for quantization, that of the boundary in configuration space, results from the requirement that spatial 3-metrics be positive definite. In general, configuration spaces with boundary require the imposition of boundary conditions on quantum states in order for the Hamiltonian operator to be self-adjoint. In the case of quantum gravity, such boundary conditions take on added interest because of their significance to the quantum behavior of the universe close to the Big Bang/Big Crunch singularity.

The ambiguities of operator ordering and boundary condition are not special to canonical quantization, but manifest themselves in a path integral approach through the choice in definition of a path integral measure and contour of paths to integrate over. The link is most readily seen by considering a (formal) path integral expression for a wave functional

$$\Psi[h_{ab}] = \mathcal{N} \int_{\mathcal{C}} e^{-I_E[g_{\alpha\beta}]} \mathcal{D}[g_{\alpha\beta}] \quad (1.3)$$

as in the Hartle–Hawking wave function of the universe [16], where \mathcal{N} represents a normalization constant, $I_E[g]$ is the Euclidean signature action evaluated on a trajectory through the superspace of metric configurations, and \mathcal{C} represents a suitable contour of 4-metrics $g_{\alpha\beta}$ bounded by the 3-metric h_{ab} at time $t = 0$. Since the wave functional (1.3) must satisfy a Wheeler–DeWitt equation for given factor ordering together with a boundary condition on superspace, and since its only variability is in the definition of the path integral measure $\mathcal{D}[g_{\alpha\beta}]$ and contour \mathcal{C} , these choices must be made jointly.

Various proposals exist to motivate the choice of particular orderings or measures on physical grounds, primarily supported by the rationale that classically reparametrization-invariant theories should retain coordinate invariance upon quantization [2, 4, 15, 23]. Reasoning along these lines has led to the arguments in favor of a Laplace–Beltrami ordering in which the kinetic term of the Hamiltonian is promoted to a covariant Laplace–Beltrami operator on configuration space. More generally, a multiple of the Ricci curvature of configuration space may be added without breaking reparametrization invariance; such an ordering is known as a conformal ordering.

An important means of illuminating the question of factor ordering is to investigate the explicit dependence of the path integral measure on the choice of ordering. The subtlety of this correspondence stems in part from the fact that rigorous definition of a path integral measure for a quantum field theory is intrinsically difficult, since one integrates over paths through a space of field configurations. In addition, two complications arise in general relativity: (1) the DeWitt supermetric (1.1) has signature $(- + + + +)$ (so that one mode always has an opposite sign in the kinetic term), and (2) the configuration space of 3-metrics g_{ab} is restricted by the requirement of positive definiteness.

In this paper, we examine the correspondence between factor orderings and path integral measures in the model problem of (1+1) gravity. As shown by Nakayama in [24], a reduction from field theory to a mechanical system is possible through gauge fixing, with no imposition of symmetries. This model facilitates a direct consideration of the boundary problem in configuration space, absent the indefinite signature in the kinetic term.

We introduce a 1-parameter family of factor orderings and demonstrate that this is equivalent to the addition of a singular quantum potential in the Hamiltonian. The mathematically rigorous construction of the Feynman path integral involving a singular potential was formulated by Nelson in [25]. Orderings which yield a potential well or sufficiently shallow barrier necessitate a boundary condition on quantum states to determine a time evolution operator; a sufficiently steep positive quantum potential obviates the need for any boundary condition on wave functions (resulting in a unique time evolution operator).

Orderings yielding a positive barrier, in concert with a Dirichlet boundary condition on quantum states, permit application of Trotter-type product formulae to express the time evolution operator as a path integral. In the critical case between a potential well and a barrier, path integral representations of time evolution under each possible boundary condition may be constructed for those orderings which yield no added quantum potential. In particular, the Laplace–Beltrami ordering (which here coincides with the conformal ordering) belongs to this class. For orderings yielding a well near the singularity, the product formulae under consideration do not apply, and the question of path integral representation remains for future investigation.

We state some supporting mathematical results in Section 2. In Section 3 a brief exposition of the model for (1+1) gravity is presented. We canonically quantize the model and introduce factor orderings in Section 4. Section 5 contains a rigorous examination of the domains of quantum states corresponding to each factor ordering in the 1-parameter family, and we derive path-integral representations of time evolution in Section 6.

2 Mathematical background

In this section we state some fundamental results used in subsequent sections. We take \mathcal{H} to be a separable Hilbert space with inner product $\langle \cdot, \cdot \rangle$. For detailed development of the functional calculus for self-adjoint operators on \mathcal{H} , we direct the reader to [29, 30]; however we state some important definitions and theorems for completeness.

Theorem 2.1 (von Neumann). *Let A be a symmetric operator on a Hilbert space \mathcal{H} . Then the following are equivalent:*

- (a) A is essentially self-adjoint.
- (b) $\text{Ker}(A^* \pm i) = \{0\}$.
- (c) $\text{Ran}(A \pm i)$ is dense in \mathcal{H} .

Every symmetric operator A has a closed extension, as A^* is always closed for densely defined operators. However there may be multiple closed extensions of A as we note below.

Definition 2.2. Suppose that A is a symmetric operator. Let

$$\mathcal{K}_{\pm} = \text{Ker}(i \mp A^*) = \text{Ran}(\pm i + A)^{\perp}.$$

\mathcal{K}_{+} and \mathcal{K}_{-} are the *deficiency subspaces* of A , and the pair of numbers n_{+} and n_{-} given by $n_{+}(A) = \dim(\mathcal{K}_{-})$ and $n_{-}(A) = \dim(\mathcal{K}_{+})$ are the *deficiency indices* of A .

As famously proven by von Neumann, the self-adjoint extensions of a closed symmetric operator bijectively correspond to partial isometries between the deficiency subspaces. In particular, considering operators of the form $\hat{H} = -\hbar^2 \frac{d^2}{dx^2} + V(x)$, we make use of a theorem due to H. Weyl.

Definition 2.3. The potential $V(x)$ is in the *limit circle case* at infinity (resp. at zero) if for some λ , all solutions of

$$-\varphi''(x) + V(x)\varphi(x) = \lambda\varphi(x)$$

are square integrable at infinity (resp. at zero). If $V(x)$ is not in the limit circle case at infinity (resp. at zero), it is said to be in the *limit point case*.

Theorem 2.4 (Weyl's limit point-limit circle criterion). *Let $V(x)$ be a continuous real-valued function on $(0, \infty)$. Then $\hat{H} = -\hbar^2 \frac{d^2}{dx^2} + V(x)$ is essentially self-adjoint on $C_0^{\infty}(0, \infty)$ if and only if $V(x)$ is in the limit point case at both zero and infinity.*

We seek to characterize the self-adjoint extensions of the Hamiltonian in terms of explicit boundary conditions. The following result appears in [13]:

Theorem 2.5. *If A is a symmetric operator on \mathcal{H} with deficiency indices (n, n) , $n \leq \infty$, if there is an n -dimensional Hilbert space \mathcal{H}_b (the “boundary space”), and if there exist two linear maps $\Gamma_1, \Gamma_2: D(A^*) \rightarrow \mathcal{H}_b$ such that for all $f_1, f_2 \in D(A^*)$,*

$$\langle A^* f_1, f_2 \rangle - \langle f_1, A^* f_2 \rangle = \langle \Gamma_1 f_1, \Gamma_2 f_2 \rangle_b - \langle \Gamma_2 f_1, \Gamma_1 f_2 \rangle_b,$$

and for any two $\Psi_1, \Psi_2 \in \mathcal{H}_b$ there exists $g \in D(A^*)$ satisfying

$$\Gamma_i g = \Psi_i, \quad i = 1, 2,$$

then there is a one-to-one correspondence between unitary maps $U \in \mathcal{U}(\mathcal{H}_b)$ and the self-adjoint extensions of A , where a map U describes the domain of the corresponding extension A_U as

$$D(A_U) = \{\psi \in D(A^*) \mid (U - 1_b)\Gamma_1\psi + i(U + 1_b)\Gamma_2\psi = 0\}.$$

The existence of the boundary space for symmetric A is proven in [13]. We apply this theory to the Hamiltonians arising from various factor orderings in Section 5.

3 Action for (1+1)-dimensional gravity

Gravity in one space and one time dimension has been considered both as a model problem for full (3+1) geometric theories of gravity and for its own importance to membrane theory. Since Einstein gravity in (1+1) has trivial dynamics, one must devise an alternative formulation for geometric gravity.

The model for (1+1) gravity considered here originates in membrane theory (see the seminal paper [28] by Polyakov), where gravity is introduced through an area-minimizing action which in the conformal gauge $g_{ab} = e^\phi \hat{g}_{ab}$ (with respect to the reference metric \hat{g}_{ab}) yields the Liouville action

$$S_L[\phi, \hat{g}] = \int_D \left[\frac{1}{4} \hat{g}^{ab} \partial_a \phi \partial_b \phi + \frac{1}{2} \phi R_{\hat{g}} + 4\Lambda e^\phi \right] d^2x.$$

Subsequent work by Verlinde [35] allows this action to be written in an arbitrary gauge.

By working in the (Euclidean signature) proper-time gauge $g_{00} = 1$, $g_{01} = g_{10} = 0$, $g_{11} = \gamma(x^0, x^1)$, Nakayama [24] obtains a reduced quantum mechanical form of Verlinde's action for the (1+1) spacetime manifold $\mathbb{R} \times S^1$ parametrized by (x^0, x^1) , $0 \leq x^1 \leq \pi$. The Euler-Lagrange equations are solved to yield a factorization of the space-space component of the metric $\gamma(x^0, x^1) = \gamma_0(x^0)\gamma_1(x^1)$. Together with the condition

$$\int_0^\pi \sqrt{\gamma_1(x^1)} dx^1 = (m+1)\pi, \quad m = 0, 1, 2, \dots,$$

this implies that the normalized spatial arc length reduces to

$$l(x^0) = \frac{1}{\pi} \int_0^\pi \sqrt{\gamma(x^0, x^1)} dx^1 = (m+1)\sqrt{\gamma_0(x^0)}.$$

Consequently, the Hamiltonian becomes

$$H_{\text{red}} \propto \frac{1}{4l(x^0)} \left(\frac{dl}{dx^0} \right)^2 - \Lambda l$$

(still in the Euclidean signature), meaning that in Lorentzian signature one may adopt the Lagrangian action

$$S[l] = \int_0^T \left[\frac{1}{4l} \dot{l}^2 - \Lambda l \right] dx^0$$

with corresponding Hamiltonian

$$H = l\Pi_l^2 + \Lambda l, \tag{3.1}$$

where the momentum conjugate to l is given by $\Pi_l = \frac{\dot{l}}{2l}$. We note that since l is invariant under reparametrizations of the coordinate x^1 , the reduced action S and the subsequent constructions below are naturally preserved by spatial re-coordinatization.

Note that in [24], a term proportional to l^{-1} is included in the reduced Hamiltonian to account for Casimir energy. Since factor ordering of the kinetic term of the quantized Hamiltonian will introduce such a term naturally (see Section 4), we regard (3.1) as the classical Hamiltonian.

4 Schrödinger quantization

A prototype for sampling the effects of factor ordering ambiguity has been to consider a family of orderings of the form (e.g., [1, 16, 22, 32])

$$\hat{H}_{(j_1, j_2, j_3)} = -\hbar^2 l^{j_1} \frac{d}{dl} l^{j_2} \frac{d}{dl} l^{j_3} + \Lambda l, \quad j_1 + j_2 + j_3 = 1, \quad (4.1)$$

where the quantized circumference operator $\hat{l}: \Psi \rightarrow l\Psi$ and its conjugate momentum operator $\hat{\Pi}_l: \Psi \rightarrow -i\hbar \frac{d\Psi}{dl}$ are variously composed.

Denoting $J_{\pm} = j_3 \pm j_1$, (4.1) is formally self-adjoint with respect to the measure $l^{J_-} dl$ on $\mathbb{R}^+ = (0, \infty)$. Transforming states and observables according to

$$\begin{aligned} L^2(\mathbb{R}^+, \mu(l)dl) &\rightarrow L^2(\mathbb{R}^+, \nu(l)dl), \\ \Psi &\mapsto \tilde{\Psi} = \left[\frac{\mu(l)}{\nu(l)} \right]^{1/2} \Psi, \\ \hat{A} &\mapsto \tilde{A} = \left[\frac{\mu(l)}{\nu(l)} \right]^{1/2} A \left[\frac{\mu(l)}{\nu(l)} \right]^{-1/2}, \end{aligned} \quad (4.2)$$

with $\mu(l) = l^{J_-}$ and $\nu(l) = l^{-1/2}$, (4.1) maps to an operator \tilde{H} which is formally self-adjoint with respect to a standard measure $l^{-1/2} dl$. Thus we have

$$\hat{H}_{(j_1, j_2, j_3)} = l^{-m} \tilde{H} l^m,$$

where $m = \frac{1}{4} + \frac{J_-}{2}$ and

$$\tilde{H} = -\hbar^2 l^{1/2} \frac{d}{dl} l^{1/2} \frac{d}{dl} + \frac{\hbar^2}{4} q l^{-1} + \Lambda l, \quad q = J_+^2 - \frac{1}{4}.$$

Normalization of states and formal self-adjointness of operators is preserved under the transformation (4.2). Note that the differential operator $l^{1/2} \frac{d}{dl} l^{1/2} \frac{d}{dl}$ is the Laplace–Beltrami operator on \mathbb{R}^+ with respect to the metric $g = (l^{-1})$, and the new effective potential $\frac{\hbar^2}{4} q l^{-1} + \Lambda l$ differs from the original potential by the singular quantum potential $\frac{\hbar^2}{4} q l^{-1}$. Thus, the Laplace–Beltrami ordering ($j_1 = \frac{1}{2} = j_2$, $j_3 = 0$) belongs to the class of orderings $|J_+| = \frac{1}{2}$, where the quantum potential vanishes.

In the parameter space (j_1, j_3) of orderings, the direction J_+ is physically significant in dictating the coefficient of the quantum potential. In contrast, J_- is insignificant, because if $J_+ = J'_+$ for two orderings (j_1, j_2, j_3) and (j'_1, j'_2, j'_3) , we have

$$\hat{H}_{(j'_1, j'_2, j'_3)} = l^{-\alpha} \hat{H}_{(j_1, j_2, j_3)} l^{\alpha}, \quad \alpha = \frac{1}{2}(J_- - J'_-).$$

A further substitution $y = 2l^{1/2}$, with $dy = l^{-1/2} dl$ and $\frac{d^2}{dy^2} = l^{1/2} \frac{d}{dl} l^{1/2} \frac{d}{dl}$, transforms the curved coordinate l to a flat one, yielding

$$\tilde{H} = -\hbar^2 \frac{d^2}{dy^2} + \hbar^2 q y^{-2} + \frac{\Lambda}{4} y^2. \quad (4.3)$$

In what follows, we denote the kinetic and potential terms of \tilde{H} as

$$\tilde{T} = -\hbar^2 \Delta = -\hbar^2 \frac{d^2}{dy^2}, \quad \tilde{V} = \hbar^2 qy^{-2} + \frac{\Lambda}{4} y^2.$$

The Hamiltonian \tilde{H} , including the singular term $\hbar qy^{-2}$, resembles radial Hamiltonians arising in nuclear physics; see, e.g., [18].

5 Self-adjoint extensions of \tilde{H}

In defining a time evolution operator, the Hamiltonian (as the infinitesimal generator) must be self-adjoint (cf. Stone's theorem in [20]). Indeed, if one chooses $D(\tilde{H}) = C_0^\infty(\mathbb{R}^+)$, standard analysis (see [12, Chapter 4]) yields that

$$D(\tilde{H}^*) = \{\psi \mid \psi, \psi' \text{ a.c. in } (0, \infty); \psi, \tilde{H}\psi \in L^2(\mathbb{R}^+)\}, \quad (5.1)$$

the so-called *natural domain* of the differential operation $\tilde{H} = -\hbar^2 \frac{d^2}{dy^2} + \hbar^2 qy^{-2} + \frac{\Lambda}{4} y^2$. In Section 5.1 we show that \tilde{H} has a unique self-adjoint extension for a large class of orderings; in Sections 5.2 and 5.3 we parametrize and characterize the self-adjoint extensions corresponding to those orderings admitting multiple extensions.

5.1 Deficiency subspaces

We proceed by determining deficiency subspaces for \tilde{H} . To compute the deficiency indices of \tilde{H} we search for solutions to

$$(\tilde{H}^* - (\pm i)I)\psi(y) = 0; \quad (5.2)$$

the solution space will be denoted by \mathcal{K}^\pm (respectively). To transform (5.2), we define the variables z and φ as follows

$$z = \frac{\sqrt{\Lambda}}{2\hbar} y^2 \quad \text{and} \quad \psi(y) = z^\beta e^{-z/2} \varphi(z),$$

where $\beta = \frac{1}{4} + \frac{|J_+|}{2}$. From this (5.2) becomes

$$z \frac{d^2 \varphi}{dz^2} + (1 + |J_+| - z) \frac{d\varphi}{dz} - \left(\frac{1 + |J_+| \pm i/(\hbar\sqrt{\Lambda})}{2} \right) \varphi(z) = 0. \quad (5.3)$$

Defining $\alpha = (1 + |J_+| \pm i/(\hbar\sqrt{\Lambda}))/2$ and $\gamma = 1 + |J_+|$, (5.3) is recognizable as the confluent hypergeometric equation

$$z \frac{d^2 \varphi}{dz^2} + (\gamma - z) \frac{d\varphi}{dz} - \alpha \varphi = 0. \quad (5.4)$$

Solutions to (5.4) are confluent hypergeometric functions of the first and second kind (respectively) [21]:

$$\begin{aligned} \varphi_1(z) &= \Phi(\alpha, \gamma; z) := \sum_{k=0}^{\infty} \frac{(\alpha)_k}{(\gamma)_k} \frac{z^k}{k!}, \\ \varphi_2(z) &= \Psi(\alpha, \gamma; z) := \frac{\Gamma(1-\gamma)}{\Gamma(1+\alpha-\gamma)} \Phi(\alpha, \gamma; z) + \frac{\Gamma(\gamma-1)}{\Gamma(\alpha)} z^{1-\gamma} \Phi(1+\alpha-\gamma, 2-\gamma; z), \end{aligned}$$

where $|z| < \infty$, $|\arg(z)| < \pi$, $\gamma \neq 0, -1, -2, \dots$, and the Pochhammer symbol $(a)_k = a(a+1)\cdots(a+k-1)$ for $a \in \mathbb{C}$ and integer $k \geq 0$. We obtain the following solutions to (5.2):

$$\begin{aligned}\psi_1^\pm(y) &= z^\beta e^{-z/2} \sum_{k=0}^{\infty} \left(\frac{1+|J_+|}{2} \pm \frac{i}{2\hbar\sqrt{\Lambda}} \right)_k \frac{z^k}{k!(1+|J_+|)_k}, \\ \psi_2^\pm(y) &= \frac{\Gamma(-|J_+|)}{\Gamma\left(\frac{1-|J_+|}{2} \pm \frac{i}{2\hbar\sqrt{\Lambda}}\right)} z^\beta e^{-z/2} \sum_{k=0}^{\infty} \left(\frac{1+|J_+|}{2} \pm \frac{i}{2\hbar\sqrt{\Lambda}} \right)_k \frac{z^k}{k!(1+|J_+|)_k} \\ &\quad + \frac{\Gamma(|J_+|)}{\Gamma\left(\frac{1+|J_+|}{2} \pm \frac{i}{2\hbar\sqrt{\Lambda}}\right)} z^{\beta-|J_+|} e^{-z/2} \sum_{k=0}^{\infty} \left(\frac{1-|J_+|}{2} \pm \frac{i}{2\hbar\sqrt{\Lambda}} \right)_k \frac{z^k}{k!(1-|J_+|)_k}.\end{aligned}$$

With the intent of applying Theorem 2.4 we investigate asymptotic behavior of these solutions for small and large y . As $y \rightarrow 0^+$,

$$\begin{aligned}\psi_1^\pm(y) &= O(y^{2\beta}) = O(y^{\frac{1}{2}+|J_+|}), \\ \psi_2^\pm(y) &= O(y^{2\beta}) + O(y^{2\beta-2|J_+|}) = O(y^{\frac{1}{2}+|J_+|}) + O(y^{\frac{1}{2}-|J_+|}) = O(y^{\frac{1}{2}-|J_+|}).\end{aligned}$$

Thus $\psi_1^\pm \in L^2$ near 0, and $\psi_2^\pm \in L^2$ near 0 precisely when $|J_+| < 1$. As in [21], for $z \rightarrow \infty$:

$$\Phi(\alpha, \gamma; z) = O(e^z z^{-(\gamma-\alpha)}), \quad \Psi(\alpha, \gamma; z) = O(z^{-\alpha}),$$

and as $y \rightarrow \infty$,

$$\psi_1^\pm(y) = O\left(e^{\frac{\sqrt{\Lambda}}{4\hbar}y^2} y^{-\frac{1}{2} \mp \frac{i}{\hbar\sqrt{\Lambda}}}\right), \quad \psi_2^\pm(y) = O\left(e^{-\frac{\sqrt{\Lambda}}{4\hbar}y^2} y^{\frac{3}{2}+2|J_+| \pm \frac{i}{\hbar\sqrt{\Lambda}}}\right).$$

Thus $\psi_1^\pm \notin L^2$ near ∞ and $\psi_2^\pm \in L^2$ near ∞ for all factor orderings. Consequently for $|J_+| \geq 1$, $\mathcal{K}^\pm = \{0\}$ and $n_+(\tilde{H}) = 0 = n_-(\tilde{H})$. For $|J_+| < 1$, $\mathcal{K}^\pm = \text{Span}\{\psi_2^\pm\}$ and $n_+(\tilde{H}) = 1 = n_-(\tilde{H})$. These analyses support the following result related to the Hamiltonian (4.3):

Theorem 5.1. *The operator $\tilde{H} = -\hbar^2 \frac{d^2}{dy^2} + \hbar^2(|J_+|^2 - \frac{1}{4})\frac{1}{y^2} + \frac{\Lambda}{4}y^2$ is essentially self-adjoint on $C_0^\infty(0, \infty)$ iff $|J_+| \geq 1$.*

Proof. We have seen that $\psi_2^\pm(y)$ is square integrable near zero iff $|J_+| < 1$. Thus, $V(y) = \hbar^2(|J_+|^2 - \frac{1}{4})\frac{1}{y^2} + \frac{\Lambda}{4}y^2$ is in limit point case at zero iff $|J_+| \geq 1$. Since $\psi_1^\pm(y)$ is never square integrable at infinity, $V(y)$ is always in limit point case at infinity. Applying Theorem 2.4 now establishes the desired result. \blacksquare

5.2 Self-adjoint extensions in terms of boundary spaces

For the case when $|J_+| < 1$, we seek to characterize and classify the self-adjoint extensions of \tilde{H} in terms of boundary conditions as in Theorem 2.5. Our method is similar to that presented in [8]. Suppose that $\tilde{\mathcal{H}}_b = \mathbb{C}$, and $\varphi^{(1)}, \varphi^{(2)}$ are solutions to $\tilde{H}\varphi = 0$ with Wronskian $W[\varphi^{(1)}, \varphi^{(2)}] = 1$ (referred to as *reference modes*). Let $\Gamma_i: D(\tilde{H}^*) \rightarrow \mathbb{C}$ be defined by

$$\Gamma_i \psi = \lim_{y \rightarrow 0^+} W[\varphi^{(i)}, \psi], \quad \text{for } i = 1, 2.$$

A straightforward computation establishes that for all $\psi_1, \psi_2 \in D(\tilde{H}^*)$,

$$\langle \tilde{H}^* \psi_1, \psi_2 \rangle - \langle \psi_1, \tilde{H}^* \psi_2 \rangle = \langle \Gamma_1 \psi_1, \Gamma_2 \psi_2 \rangle_{\mathbb{C}} - \langle \Gamma_2 \psi_1, \Gamma_1 \psi_2 \rangle_{\mathbb{C}},$$

and for any $\Psi_1, \Psi_2 \in \mathbb{C}$, one may construct $g \in D(\tilde{H}^*)$ (by choosing $g_{1,2} \sim C_{1,2}y^{\pm 2\nu + \frac{1}{2}}$ and taking $g = g_1 + g_2$) satisfying that $\Gamma_i g = \Psi_i$, $i = 1, 2$.

To determine an explicit formula for the reference modes, we write

$$\tilde{H}\varphi = -\hbar^2\varphi''(y) + \left(\frac{\hbar^2q}{y^2} + \frac{\Lambda y^2}{4}\right)\varphi(y) = 0,$$

where, as before, $q = J_+^2 - \frac{1}{4}$. Making the substitutions $w(y) = \frac{\sqrt{\Lambda}}{4\hbar}y^2$ and $\varphi(y) = w^{1/4}u(w)$ we obtain

$$w^2u''(w) + wu'(w) - \left(w^2 + \left(\frac{J_+}{2}\right)^2\right)u(w) = 0.$$

This is a modified Bessel equation; letting $\nu = \frac{|J_+|}{2}$, solutions to this equation are given by the modified Bessel functions of the first ($I_\nu(w)$) and second ($K_\nu(w)$) kind; their Wronskian satisfies $W[K_\nu(w), I_\nu(w)] = 1/w$. Choosing

$$\varphi^{(1)}(y) = \frac{\sqrt{y}}{\sqrt{2}}K_\nu\left(\frac{\sqrt{\Lambda}}{4\hbar}y^2\right) \quad \text{and} \quad \varphi^{(2)}(y) = \frac{\sqrt{y}}{\sqrt{2}}I_\nu\left(\frac{\sqrt{\Lambda}}{4\hbar}y^2\right),$$

it follows that $W[\varphi^{(1)}, \varphi^{(2)}] = 1$.

The asymptotic equivalences (for $w \rightarrow 0$) of modified Bessel functions are well-known:

$$K_\nu(w) \sim \begin{cases} \frac{\pi}{2} \frac{1}{\sin(\nu\pi)} \frac{1}{\Gamma(1-\nu)} \left(\frac{w}{2}\right)^{-\nu}, & \nu \notin \mathbb{Z}, \\ -\ln\left(\frac{w}{2}\right), & \nu = 0, \end{cases} \quad I_\nu(w) \sim \frac{1}{\Gamma(\nu+1)} \left(\frac{w}{2}\right)^\nu.$$

These yield

$$\varphi^{(1)}(y) \sim \begin{cases} \mathcal{C}_1 y^{-2\nu+\frac{1}{2}}, & 0 < |J_+| < 1, \\ -\sqrt{2}y^{1/2} \ln y + ky^{1/2}, & J_+ = 0, \end{cases} \quad (5.5)$$

where

$$\mathcal{C}_1 = \frac{\pi}{2\sqrt{2}} \frac{1}{\sin(\nu\pi)} \left(\frac{\sqrt{\Lambda}}{8\hbar}\right)^{-\nu} \frac{1}{\Gamma(1-\nu)}, \quad k = -\frac{1}{\sqrt{2}} \ln\left(\frac{\sqrt{\Lambda}}{8\hbar}\right),$$

and

$$\varphi^{(2)}(y) \sim \mathcal{C}_2 y^{2\nu+\frac{1}{2}}, \quad (5.6)$$

where

$$\mathcal{C}_2 = \frac{1}{\sqrt{2}} \frac{1}{\Gamma(\nu+1)} \left(\frac{\sqrt{\Lambda}}{8\hbar}\right)^\nu.$$

The corresponding asymptotic behavior of the derivatives is given by

$$\begin{aligned} \varphi^{(1)'}(y) &\sim \begin{cases} (-2\nu + \frac{1}{2}) \mathcal{C}_1 y^{-2\nu-\frac{1}{2}}, & 0 < |J_+| < 1, \\ -\frac{1}{\sqrt{2}} y^{-1/2} \ln y + \left(\frac{k}{2} - \sqrt{2}\right) y^{-1/2}, & J_+ = 0, \end{cases} \\ \varphi^{(2)'}(y) &\sim (2\nu + \frac{1}{2}) \mathcal{C}_2 y^{2\nu-\frac{1}{2}}. \end{aligned}$$

For detailed treatment of modified Bessel functions and asymptotic behavior we direct the reader to [21]. Let $\xi \in U(1)$ and $\psi \in D(\tilde{H}^*)$. Writing $L = \tan(\arg(\xi)/2)$ we have, for $0 < |J_+| < 1$:

$$\begin{aligned} & (\xi - 1)\Gamma_1\psi + i(\xi + 1)\Gamma_2\psi \\ &= \lim_{y \rightarrow 0^+} \psi(y) [L(2\beta - 1)\mathcal{C}_1 y^{-2\beta} - 2\beta\mathcal{C}_2 y^{2\beta-1}] + \psi'(y) [L\mathcal{C}_1 y^{1-2\beta} + \mathcal{C}_2 y^{2\beta}], \end{aligned} \quad (5.7)$$

where as before, $\beta = \frac{1}{4} + \frac{|J_+|}{2}$. For $|J_+| = 0$ we have

$$\begin{aligned} & (\xi - 1)\Gamma_1\psi + i(\xi + 1)\Gamma_2\psi \\ &= \lim_{y \rightarrow 0^+} \frac{\psi(y)}{\sqrt{y}} [L(\sqrt{2}\ln(y) - \frac{k}{2} + \sqrt{2}) - \frac{1}{2}\mathcal{C}_2] + \psi'(y)\sqrt{y} [L(-\sqrt{2}\ln(y) + k) + \mathcal{C}_2]. \end{aligned} \quad (5.8)$$

The self-adjoint extensions of \tilde{H} are parametrized by $L \in (-\infty, \infty]$ and may thus be characterized as the restriction of \tilde{H}^* to functions in $D(\tilde{H}^*)$ such that the limits in (5.7) and (5.8) (for respective values of $|J_+|$) are zero.

5.3 Self-adjoint extensions in terms of asymptotics

An alternate approach to characterizing self-adjoint domains for \tilde{H} involves describing the asymptotic behavior of functions in the natural domain (5.1) of \tilde{H} and imposing restrictions which force $\lim_{\varepsilon \rightarrow 0^+} \lim_{L \rightarrow \infty} (\bar{\psi}'\psi - \bar{\psi}\psi')|_{\varepsilon}^L = 0$. Combined with the polarization identity, such a restriction causes the integration-by-parts terms obstructing self-adjointness of \tilde{H} to vanish (see, e.g., [12, Section 3.2]).

The asymptotic analysis of the natural domain is accomplished by applying methods similar to those used by Gitman et al. [11, 12] for the Calogero problem. The condition $\tilde{H}\psi \in L^2(\mathbb{R}^+)$ effectively describes each $\psi \in D(\tilde{H}^*)$ as the solution of some differential equation

$$\tilde{H}\psi = \chi, \quad \chi \in L^2(\mathbb{R}^+). \quad (5.9)$$

The general solution to (5.9) can be written in terms of the reference modes $\varphi^{(1)}, \varphi^{(2)}$ as

$$\begin{aligned} \psi &= c_1\varphi^{(1)} + c_2\varphi^{(2)} + \tilde{\psi}, \quad c_1, c_2 \in \mathbb{C}, \\ \tilde{\psi} &= \frac{1}{\hbar^2} \left[\varphi^{(1)} \int_{a_2}^y \chi \varphi^{(2)} dy' - \varphi^{(2)} \int_{a_1}^y \chi \varphi^{(1)} dy' \right], \end{aligned} \quad (5.10)$$

since a straightforward computation verifies that $\tilde{\psi}$ is a particular solution to (5.9).

Utilizing the asymptotic behavior of the reference modes (5.5), (5.6) (valid for all values of $|J_+|$, with minor adjustment to coefficients) and applying the Cauchy–Schwarz inequality yields

$$\int_{a_1}^y \chi \tilde{\psi}_1 dy' = \begin{cases} O(y^{-|J_+|+1}), & |J_+| \neq 1, \\ O(\sqrt{\ln(y)}), & |J_+| = 1, \end{cases} \quad \int_{a_2}^y \chi \tilde{\psi}_2 dy' = O(y^{|J_+|+1}). \quad (5.11)$$

For $|J_+| \neq 0$, we have that when $|J_+| \neq 1$, $\tilde{\psi} = O(y^{3/2})$ and $\tilde{\psi}' = O(y^{1/2})$; when $|J_+| = 1$, $\tilde{\psi} = O(y^{3/2} \ln(y))$ and $\tilde{\psi}' = O(y^{1/2} \ln(y))$.

For $J_+ = 0$, we apply analogous asymptotics (relying upon a series relation between $K_0(w)$ and $I_0(w)$ (see, e.g., [26])):

$$K_0(w(y)) = -\ln\left(\frac{w(y)}{2}\right) I_0(w(y)) + \sum_{k=0}^{\infty} \frac{w(y)^{2k}}{2^k (k!)^2} \Psi(k+1) = -2[\ln(y)I_0(w(y)) + R(y)],$$

where

$$R(y) = \frac{1}{2} \left[\ln \left(\frac{\sqrt{\Lambda}}{8\hbar} \right) I_0(w(y)) - \sum_{k=0}^{\infty} \frac{w(y)^{2k}}{2^k (k!)^2} \Psi(k+1) \right],$$

and Ψ is the digamma function $\Psi(x) = \frac{d}{dx}[\ln(\Gamma(x))]$. Note that $R(y) = O(1)$ as $y \rightarrow 0$. Thus we can write (taking $a_1 = 0 = a_2$)

$$\begin{aligned} \tilde{\psi}(y) = & -\frac{\sqrt{y}}{\hbar^2} I_0(w(y)) \left[\ln y \int_0^y \chi(y') \sqrt{y'} I_0(z(y')) dy' - \int_0^y \chi(y') \sqrt{y'} \ln(y') I_0(w(y')) dy' \right] \\ & - \frac{\sqrt{y}}{\hbar^2} \left[R(y) \int_0^y \chi(y') \sqrt{y'} I_0(w(y')) dy' - I_0(w(y)) \int_0^y \chi(y') \sqrt{y'} R(y') dy' \right]. \end{aligned} \quad (5.12)$$

To simplify the asymptotic analysis of (5.12) as $y \rightarrow 0$, define

$$\Theta(y) = \int_0^y \chi(y') \sqrt{y'} I_0(w(y')) dy', \quad \Theta'(y) = \chi(y) \sqrt{y} I_0(w(y)),$$

and use the Cauchy–Schwartz inequality as in (5.11) to obtain $\Theta(y) = O(y)$ as $y \rightarrow 0$. We can now use integration by parts to rewrite (5.12) as

$$\begin{aligned} \tilde{\psi}(y) = & \frac{\sqrt{y}}{\hbar^2} I_0(w(y)) \left[\int_0^y \ln(y') \Theta'(y') dy' - \ln y \Theta(y) \right] \\ & + \frac{\sqrt{y}}{\hbar^2} \left[I_0(w(y)) \int_0^y \chi(y') \sqrt{y'} R(y') dy' - R(y) \int_0^y \chi(y') \sqrt{y'} I_0(w(y')) dy' \right] \\ = & -\frac{\sqrt{y}}{\hbar^2} I_0(w(y)) \int_0^y \frac{1}{y'} \Theta(y') dy' \\ & + \frac{1}{\hbar^2} \left[A(y) \int_0^y \chi(y') B(y') dy' - B(y) \int_0^y \chi(y') A(y') dy' \right], \end{aligned} \quad (5.13)$$

where for simplicity $A(y) = \sqrt{y} I_0(w(y))$ and $B(y) = \sqrt{y} R(y)$. Using the fact that $\Theta(y) = O(y)$ and $R(y) = O(1)$, we can once again apply the Cauchy–Schwartz inequality to derive the asymptotic estimates

$$\int_0^y \chi A dy' = O(y) = \int_0^y \chi B dy',$$

so that $\tilde{\psi} = O(y^{3/2})$. Differentiating (5.13) and applying similar asymptotic analysis yields $\tilde{\psi}' = O(y^{1/2})$.

When $|J_+| \geq 1$, \tilde{H} is essentially self-adjoint. Indeed, in this case, (5.10) implies $c_1 = 0$ since $\psi \in L^2(\mathbb{R}^+)$; furthermore, the term $c_2 \varphi^{(2)}$ is absorbed into the asymptotic term corresponding to $\tilde{\psi}$, permitting no freedom in the choice of self-adjoint domain.

When \tilde{H} is not essentially self-adjoint (i.e., when $|J_+| < 1$), a 1-parameter family of pairs (c_1, c_2) indexes the set of self-adjoint extensions. We determine the self-adjoint domains for \tilde{H} by requiring that $\lim_{\varepsilon \rightarrow 0^+} \lim_{L \rightarrow \infty} (\overline{\psi'} \psi - \overline{\psi} \psi')|_{\varepsilon}^L = 0$, or, since $\lim_{L \rightarrow \infty} \psi(L) = 0$ and $\lim_{L \rightarrow \infty} \psi'(L) = 0$, that $\lim_{\varepsilon \rightarrow 0} (\overline{\psi'} \psi - \overline{\psi} \psi')|_{\varepsilon} = 0$. The asymptotic equivalences for $0 < |J_+| < 1$

$$\begin{aligned} \psi & \sim c_1 \mathcal{C}_1 y^{-|J_+| + \frac{1}{2}} + c_2 \mathcal{C}_2 y^{|J_+| + \frac{1}{2}} + O(y^{\frac{3}{2}}), \\ \psi' & \sim c_1 \mathcal{C}_1 (-|J_+| + \frac{1}{2}) y^{-|J_+| - \frac{1}{2}} + c_2 \mathcal{C}_2 (|J_+| + \frac{1}{2}) y^{|J_+| - \frac{1}{2}} + O(y^{\frac{1}{2}}) \end{aligned}$$

imply that $\lim_{\varepsilon \rightarrow 0} (\bar{\psi}'\psi - \bar{\psi}\psi')|_\varepsilon = -2|J_+|\mathcal{C}_1\mathcal{C}_2(\bar{c}_1c_2 - c_1\bar{c}_2)$, so we must require $\bar{c}_1c_2 - c_1\bar{c}_2 = 0$ to obtain a domain on which \tilde{H} is self adjoint. For orderings satisfying $J_+ = 0$, we have instead the asymptotic equivalences

$$\begin{aligned}\psi &\sim c_1(-\sqrt{2}y^{\frac{1}{2}}\ln(y) - ky^{\frac{1}{2}}) + c_2\mathcal{C}_2y^{\frac{1}{2}} + O(y^{\frac{3}{2}}), \\ \psi' &\sim c_1(-\frac{1}{\sqrt{2}}y^{-\frac{1}{2}}\ln(y) + (\frac{k}{2} - \sqrt{2})y^{-\frac{1}{2}}) + c_2\frac{1}{2}\mathcal{C}_2y^{-\frac{1}{2}} + O(y^{\frac{1}{2}}),\end{aligned}$$

where as before, $k = -\frac{1}{\sqrt{2}}\ln(\frac{\sqrt{\Lambda}}{8h})$. These similarly yield $\lim_{\varepsilon \rightarrow 0} (\bar{\psi}'\psi - \bar{\psi}\psi')|_\varepsilon = -\sqrt{2}\mathcal{C}_2(\bar{c}_1c_2 - c_1\bar{c}_2)/\hbar$. Thus $\bar{c}_1c_2 = c_1\bar{c}_2$, implying $\bar{c}_1c_2 \in \mathbb{R}$, and hence c_2 is a real multiple of c_1 , since

$$\alpha c_1 = (\bar{c}_2c_1)c_1 = (\bar{c}_1c_2)c_1 = (\bar{c}_1c_1)c_2 = \beta c_2, \quad \alpha, \beta \in \mathbb{R}.$$

Note that we can define θ such that $\tan \theta = \frac{\beta}{\alpha}$, yielding $c_1 \cos(\theta) = c_2 \sin(\theta)$, and allowing us to write ψ in the form

$$\psi = C(\sin(\theta)\varphi^{(1)} + \cos(\theta)\varphi^{(2)}) + O(y^{\frac{3}{2}}), \quad (5.14)$$

implying the asymptotics

$$\psi \sim \begin{cases} C(\sin(\theta)\mathcal{C}_1y^{-|J_+|+\frac{1}{2}} + \cos(\theta)\mathcal{C}_2y^{|J_+|+\frac{1}{2}}) + O(y^{\frac{3}{2}}), & 0 < |J_+| < 1, \\ C(\sin(\theta)(-\sqrt{2}y^{\frac{1}{2}}\ln(y) + ky^{\frac{1}{2}}) + \cos(\theta)\mathcal{C}_2y^{\frac{1}{2}}) + O(y^{\frac{3}{2}}), & |J_+| = 0, \end{cases} \quad (5.15)$$

and similarly for ψ' . Taking $\theta = \tan^{-1}(L)$ we observe that this parametrization of the self-adjoint extensions for \tilde{H} may be recast in the form as in (5.7) and (5.8).

6 Formulation of the propagator and path-integral representation of the fundamental solution

In this section, we use extensions of the Trotter product formula due to Kato and to Exner, Neidhardt, and Zagrebnov to derive Feynman-Kač formulae (i.e., path integral representations) for the time-evolution operators $e^{-it\tilde{H}/\hbar}$ and $e^{-t\tilde{H}/\hbar}$ evolving initial data according to the real- and imaginary-time Schrödinger equations, respectively. By factoring the time evolution operator $\mathcal{U}_t = e^{-at\tilde{H}/\hbar}$ ($a = i, 1$) as the limit of the concatenation of short-time evolution operators $(e^{-at\tilde{T}/\hbar n} e^{-at\tilde{V}/\hbar n})^n$, we can write a path-integral expression for the propagator (integral kernel) of $e^{-at\tilde{H}} = e^{-at(\tilde{T}+\tilde{V})}$ by using the known integral kernel for $e^{-at\tilde{T}/\hbar n} = e^{a\hbar t\Delta/n}$.

The Trotter product formula and its extensions require that the operators \tilde{T} and \tilde{V} be self-adjoint [14], so the domain of $\tilde{T} = -\hbar^2 \frac{d^2}{dy^2}$ must correspond to one of the self-adjoint extensions of the Laplacian on the half-line; namely, \tilde{T} must be taken to be \tilde{T}_β , $\beta \in (-\infty, \infty]$, where

$$\begin{aligned}\tilde{T}_\beta &= -\hbar^2 \Delta = -\hbar^2 \frac{d^2}{dy^2}, \\ D(\tilde{T}_\beta) &= \{ \psi \in D_T^* \mid \lim_{\varepsilon \rightarrow 0} [\psi(\varepsilon) - \beta\psi'(\varepsilon)] = 0 \}\end{aligned}$$

(as usual, $\beta = \infty$ denotes the Neumann boundary condition $\psi'(0) = 0$).

The familiar Trotter product formula further requires that $\tilde{H} = \tilde{T}_\beta + \tilde{V}$ be essentially self-adjoint on $D(\tilde{T}_\beta) \cap D(\tilde{V})$, a problematic condition in the presence of multiple self-adjoint extensions of \tilde{H} for $|J_+| < 1$. The extended results of Kato and of Exner et al do not require essential self-adjointness of $\tilde{T}_\beta + \tilde{V}$, but instead demand that \tilde{T}_β and \tilde{V} be nonnegative.

Consequently their application is limited to factor orderings such that $|J_+| \geq \frac{1}{2}$ and hence $V(y) = \hbar^2(|J_+|^2 - \frac{1}{4})\frac{1}{y^2} + \frac{\Lambda}{4}y^2 \geq 0$.

The following subsections construct Feynman–Kač formulas in real and imaginary time, for the cases $|J_+| \geq \frac{1}{2}$. The case $|J_+| = \frac{1}{2}$ is special because for such factor orderings, the quantum potential term $\hbar q y^{-2} = \hbar(J_+^2 - \frac{1}{4})y^{-2}$ in $V(y)$ vanishes. For $|J_+| < \frac{1}{2}$, neither the standard Trotter product formula nor extensions due to Kato and to Exner et al apply. In the case of the extensions, the operator \tilde{V} fails to be nonnegative, while the standard Trotter product theorem does not apply since $D(\tilde{T}_\beta) \cap D(\tilde{V})$ does not determine one of the self-adjoint extensions of \tilde{H} . Indeed, functions $\psi \in D(\tilde{V})$ satisfy

$$\int_0^\infty y^{-4}|\psi|^2 dy < \infty, \quad (6.1)$$

while elements of the self-adjoint extension of \tilde{H} corresponding to the angle θ in $\text{Span}\{\varphi^{(1)}, \varphi^{(2)}\}$ behave asymptotically as (5.15) near $y = 0$. For $|J_+| < \frac{1}{2}$, the condition (6.1) can only be satisfied when $C = 0$, meaning that $D(\tilde{T}_\beta) \cap D(\tilde{V})$ satisfies the boundary conditions of all self-adjoint extensions of \tilde{H} , and thus \tilde{H} is not essentially self-adjoint on $D(\tilde{T}_\beta) \cap D(\tilde{V})$. In fact, (6.1) can only be satisfied when $C = 0$ for all $|J_+| < 1$ (where $|J_+| \neq \frac{1}{2}$, since at $|J_+| = \frac{1}{2}$ (6.1) does not apply), so the standard Trotter product formula is inapplicable for all such orderings.

Complementary to the path integral approach to constructing a time evolution operator one may use spectral decomposition of the Hamiltonian to define propagators as in [27].

6.1 Imaginary-time Feynman–Kač formula

6.1.1 Factor orderings with $|J_+| > \frac{1}{2}$

For factor orderings in this range, both \tilde{T}_β and \tilde{V} are nonnegative self-adjoint operators. In addition, the intersection of their form domains $Q(\tilde{T}_\beta) \cap Q(\tilde{V})$ (equivalently, $D(\tilde{T}_\beta^{1/2}) \cap D(\tilde{V}^{1/2})$) is dense (since it contains $C_0^\infty(\mathbb{R}^+)$). Thus the operators \tilde{T}_β and \tilde{V} satisfy the hypotheses of the strong Kato–Trotter product formula (see, e.g., [29, Theorem S.21]). We conclude that the quadratic form $\langle \varphi, \tilde{T}_\beta \psi \rangle_{L^2(\mathbb{R}^+)} + \langle \varphi, \tilde{V} \psi \rangle_{L^2(\mathbb{R}^+)}$ is closed on the domain $Q(\tilde{T}_\beta) \cap Q(\tilde{V})$, and hence is associated with a self-adjoint operator, denoted $\tilde{T}_\beta \dot{+} \tilde{V}$ (the *form sum* of \tilde{T}_β and \tilde{V}). The product formula

$$e^{-t(\tilde{T}_\beta \dot{+} \tilde{V})} = \text{s-lim}_{n \rightarrow \infty} (e^{-t\tilde{T}_\beta/n} e^{-t\tilde{V}/n})^n \quad (6.2)$$

then holds.

We first investigate the domain $D(\tilde{T}_\beta \dot{+} \tilde{V}) \subseteq Q(\tilde{T}_\beta) \cap Q(\tilde{V})$ for the self-adjoint operator $\tilde{T}_\beta \dot{+} \tilde{V}$. Observe that since

$$Q(\tilde{V}) = \left\{ \psi \in L^2(\mathbb{R}^+) \mid \int_0^\infty V(y)|\psi(y)|^2 dy < \infty \right\},$$

every element $\psi \in D(\tilde{T}_\beta \dot{+} \tilde{V})$ must satisfy

$$\int_0^\infty y^{-2}|\psi(y)|^2 dy < \infty. \quad (6.3)$$

For $|J_+| \geq 1$, there is only one self-adjoint domain for \tilde{H} , and the asymptotic analysis of Section 5.3 implies that the elements satisfy $\psi \sim O(y^{\frac{3}{2}})$ near $y = 0$, consistent with (6.3); indeed, $D(\tilde{T}_\beta \dot{+} \tilde{V})$ must coincide with the single self-adjoint extension of \tilde{H} (for all values of β). For $\frac{1}{2} < |J_+| < 1$, the self-adjoint extensions of \tilde{H} are indexed by one-dimensional subspaces of

$\text{Span}\{\varphi^{(1)}, \varphi^{(2)}\}$, with each subspace determined by θ as in (5.14), so that elements of $D(\tilde{T}_\beta \dot{+} \tilde{V})$ must be characterized by a particular angle $\theta = \theta'$. Combining (6.3) and (5.14), we obtain

$$\int_0^1 y^{-2} [\sin(\theta')\varphi^{(1)}(y) + \cos(\theta')\varphi^{(2)}(y)]^2 dy < \infty. \quad (6.4)$$

Since $\varphi^{(1)} \sim \mathcal{C}_1 y^{-|J_+|+\frac{1}{2}}$, $\varphi^{(2)} \sim \mathcal{C}_2 y^{|J_+|+\frac{1}{2}}$, (6.4) can only be satisfied if $\theta' = 0$, identifying $\tilde{T}_\beta \dot{+} \tilde{V}$ as the self-adjoint extension of \tilde{H} purely in $\text{Span}\{\varphi^{(2)}\}$ (for all β).

For $|J_+| > \frac{1}{2}$ the conditions of the Kato–Trotter product formula identify a single self-adjoint extension of \tilde{H} for which one may construct a time-sliced path integral, regardless of the choice of \tilde{T}_β . Thus without loss of generality we fix \tilde{T}_0 (corresponding to the Dirichlet boundary condition on the Laplacian) as the self-adjoint extension for \tilde{T} .

We now combine the Kato–Trotter product formula with the well-known Dirichlet heat kernel on \mathbb{R}^+ (see, e.g., [3, 6, 31]) to construct a Feynman–Kač formula for the imaginary-time evolution operator $e^{-t\tilde{H}/\hbar}$ (guaranteed by the spectral theorem to be well-defined for self-adjoint \tilde{H}). The Dirichlet heat kernel on the half-line, given by

$$p_+^D(t, y, z) = \frac{1}{\sqrt{4\pi t}} [e^{-(y-z)^2/4t} - e^{-(y+z)^2/4t}], \quad (6.5)$$

is the integral kernel for $e^{t\Delta_0}$, and may be obtained by applying the ordinary heat kernel on \mathbb{R} to an odd extension of data $\psi : \mathbb{R}^+ \rightarrow \mathbb{C}$ (with $\psi(0) = 0$). The heat kernel (6.5) preserves the Dirichlet boundary condition for all time. From (6.2) and (6.5), we obtain

$$\begin{aligned} e^{-t\tilde{H}/\hbar}\psi &= \lim_{n \rightarrow \infty} (e^{-t\tilde{T}_0/\hbar n} e^{-tV(y)/\hbar n})^n \psi = \lim_{n \rightarrow \infty} (e^{\hbar t \Delta/n} e^{-tV(y)/\hbar n})^n \psi \\ &= \lim_{n \rightarrow \infty} \mathcal{N} \int_{\mathbb{R}^+} \cdots \int_{\mathbb{R}^+} \prod_{j=1}^n \left[\left(e^{-\frac{n(z_{j+1}-z_j)^2}{4\hbar t}} - e^{-\frac{n(z_{j+1}+z_j)^2}{4\hbar t}} \right) e^{-\frac{tV(z_j)}{\hbar n}} \right] \psi(z_1) dz_1 \cdots dz_n, \\ \mathcal{N} &= \left(\frac{n}{4\pi\hbar t} \right)^{n/2}. \end{aligned} \quad (6.6)$$

The path integrals corresponding to different factor orderings are distinguished by the quantum potential $\hbar^2 q y^{-2} = \hbar^2 (J_+^2 - \frac{1}{4}) y^{-2}$, so that we may write the factor

$$\prod_{j=1}^n e^{-tV(z_j)/\hbar n} = \prod_{j=1}^n e^{-t\Lambda z_j^2/4\hbar n} \prod_{k=1}^n e^{-\hbar q z_k^{-2}/n}$$

and regard the latter product on the right-hand side as a weight on the path integral measure corresponding to the factor ordering chosen. Notice that this weight is small for histories tarrying near the singularity $y = 0$. A large value of q in the quantum potential intensifies this effect.

The n -fold time-sliced measure

$$\left(\frac{n}{4\pi\hbar t} \right)^{n/2} \prod_{j=1}^n \left(e^{-\frac{n(z_{j+1}-z_j)^2}{4\hbar t}} - e^{-\frac{n(z_{j+1}+z_j)^2}{4\hbar t}} \right) dz_1 \cdots dz_n$$

represents an *avoiding measure* supported on paths away from the singularity $y = 0$. As discussed by Farhi and Gutmann in [6], the first term of (6.5) is the heat kernel for propagation from $z > 0$ to $y > 0$ on \mathbb{R} , but to construct an avoiding measure on the half-line \mathbb{R}^+ , this must be adjusted by subtracting the weight for paths from $y > 0$ to $z > 0$ incident on the origin. The appropriate weight to subtract is precisely the second term of (6.5), because paths from $y > 0$ to $z > 0$ intersecting the origin are in one-to-one correspondence with paths from y to $-z$ (for a full treatment, refer to [6, Section 2].)

We conclude that by introducing a quantum potential, factor orderings in the range $|J_+| \geq 1$ require that the path integral measure be supported on paths avoiding the singularity. A larger value of q results in a decreased contribution by histories for which the circumference of the universe remains mostly small. For orderings with $\frac{1}{2} < |J_+| < 1$, the extended product formulae limit the construction of a time-sliced path integral to one whose measure is supported on paths avoiding the singularity.

6.1.2 Factor orderings with $|J_+| = \frac{1}{2}$

As in the preceding section \tilde{T}_β and \tilde{V} are nonnegative self-adjoint operators with $Q(\tilde{T}_\beta) \cap Q(\tilde{V})$ dense, so that once again the hypotheses of the strong Kato–Trotter product formula are satisfied, for $\beta \in (-\infty, \infty]$. Thus $\tilde{T}_\beta \dot{+} \tilde{V}$ is self-adjoint on $D(\tilde{T}_\beta \dot{+} \tilde{V}) \subseteq Q(\tilde{T}_\beta) \cap Q(\tilde{V})$, and the product formula (6.2) holds.

We wish to identify $D(\tilde{T}_\beta \dot{+} \tilde{V})$ as one of the self-adjoint extensions of \tilde{H} , corresponding to θ in $\text{Span}\{\varphi^{(1)}, \varphi^{(2)}\}$. However, the absence of the quantum potential (since $q = J_+^2 - \frac{1}{4} = 0$) removes the condition (6.3); membership of ψ in $Q(\tilde{V})$ no longer imposes any restriction on asymptotics near $y = 0$, and instead we utilize that $D(\tilde{T}_\beta) \cap D(\tilde{V}) \subseteq D(\tilde{T}_\beta \dot{+} \tilde{V})$ (see, e.g., [7, Proposition 3.1]). Thus the corresponding self-adjoint extension of \tilde{H} contains elements satisfying the boundary condition $\psi(0) = \beta\psi'(0)$. Since the asymptotic analysis of Section 5.3 yields (for $|J_+| = \frac{1}{2}$),

$$\begin{aligned}\psi &\sim C(\mathcal{C}_1 \sin(\theta) + \mathcal{C}_2 \cos(\theta)y) + O(y^{3/2}), \\ \psi' &\sim C(\mathcal{C}_2 \cos(\theta)) + O(y^{1/2}),\end{aligned}\tag{6.7}$$

we conclude that β determining the self-adjoint extension of the Laplacian is related to θ for the self-adjoint extension of \tilde{H} by

$$\beta = \frac{\mathcal{C}_1}{\mathcal{C}_2} \tan \theta.\tag{6.8}$$

The Dirichlet boundary condition $\beta = 0$ corresponds to $\theta = 0$, and as in the preceding section, we use (6.5) with the Kato–Trotter product formula to obtain the same time-sliced path integral expression for $e^{-t\tilde{H}/\hbar}$ (cf. (6.6)).

The Neumann boundary condition $\psi'(0) = 0$ (formally $\beta = \infty$) corresponds to $\theta = \frac{\pi}{2}$. In this case $e^{-t\tilde{T}_\infty/n}$ in (6.2) may be expressed in terms of the well-known Neumann heat kernel on \mathbb{R}^+ (see, e.g., [3, 6, 9, 31]):

$$p_+^N(t, y, z) = \frac{1}{\sqrt{4\pi t}} [e^{-(y-z)^2/4t} + e^{-(y+z)^2/4t}],\tag{6.9}$$

derived by evenly extending data on \mathbb{R}^+ (with $\psi'(0) = 0$) to \mathbb{R} and evolving via the ordinary heat kernel. Similarly to the case for Dirichlet boundary conditions, we combine (6.9) with the Kato–Trotter product formula to obtain the time-sliced path integral propagator:

$$\begin{aligned}e^{-t\tilde{H}/\hbar}\psi &= \lim_{n \rightarrow \infty} (e^{-t\tilde{T}_\infty/\hbar n} e^{-tV(y)/\hbar n})^n \psi = \lim_{n \rightarrow \infty} (e^{\hbar t \Delta/n} e^{-tV(y)/\hbar n})^n \psi \\ &= \lim_{n \rightarrow \infty} \mathcal{N} \int_{\mathbb{R}^+} \cdots \int_{\mathbb{R}^+} \prod_{j=1}^n \left[\left(e^{\frac{-n(z_{j+1}-z_j)^2}{4\hbar t}} + e^{\frac{-n(z_{j+1}+z_j)^2}{4\hbar t}} \right) e^{\frac{-tV(z_j)}{\hbar n}} \right] \psi(z_1) dz_1 \cdots dz_n, \\ \mathcal{N} &= \left(\frac{n}{4\pi \hbar t} \right)^{n/2}.\end{aligned}$$

In contrast to the singularity-avoiding measure generated by the Dirichlet heat kernel, the Neumann n -fold time-sliced measure

$$\left(\frac{n}{4\pi \hbar t} \right)^{n/2} \prod_{j=1}^n \left(e^{\frac{-n(z_{j+1}-z_j)^2}{4\hbar t}} + e^{\frac{-n(z_{j+1}+z_j)^2}{4\hbar t}} \right) dz_1 \cdots dz_n$$

corresponds to a *reflecting measure* supported on paths which may strike the singularity on multiple occasions. As discussed in [6], the first term in (6.9) yields the weight for paths striking the origin an even number of times, since these paths are in one-to-one correspondence with paths from $y > 0$ to $z > 0$ in the whole line. The second term in (6.9) supplements the first by weighting paths which strike the origin an odd number of times, since the same correspondence associates such paths with paths in the whole line from $y > 0$ to $-z < 0$.

We have derived path integral representations for the imaginary-time evolution operators corresponding to two of the self-adjoint extensions of \tilde{H} ($\theta = 0$ and $\theta = \frac{\pi}{2}$) when $|J_+| = \frac{1}{2}$, by using the heat kernel for Dirichlet and Neumann boundary conditions, respectively. For the remaining extensions, the heat kernel for the boundary condition $\psi(0) = \beta\psi'(0)$ may be constructed using spectral decomposition of $-\Delta$ with corresponding boundary behavior. The resulting eigenfunctions are $\psi_p(y) = \left(\frac{2}{\pi}\right)^{1/2} \cos(py + \phi_p)$, where $\tan \phi_p = -1/p\beta$ (see [3, 6, 9]), yielding the heat kernel

$$p_+^{(\beta)}(t, y, z) = \frac{1}{\sqrt{4\pi t}} [e^{-(y-z)^2/4t} + e^{-(y+z)^2/4t}] - \beta^{-1} \exp\left\{\frac{t}{\beta^2} + \frac{(y+z)}{\beta}\right\} \operatorname{erfc}\left[\left(\frac{t}{\beta^2}\right)^{1/2} + \left(\frac{y+z}{2\beta}\right)\left(\frac{t}{\beta^2}\right)^{-1/2}\right].$$

The term containing the complementary error function $\operatorname{erfc}(\cdot)$ decreases as β ranges from 0 to ∞ , and may be regarded as interpolating between the avoiding and reflecting measures.

The time-sliced path integral expression for the imaginary-time evolution operator may thus be constructed as

$$e^{-t\tilde{H}/\hbar}\psi = \lim_{n \rightarrow \infty} \int_{\mathbb{R}^+} \cdots \int_{\mathbb{R}^+} \prod_{j=1}^n \left[p_+^{(\beta)}\left(\frac{\hbar t}{n}, z_{j+1}, z_j\right) e^{-tV(z_j)/\hbar n} \right] \psi(z_1) dz_1 \cdots dz_n.$$

6.2 Real-time Feynman–Kac formula

The Trotter product formula for real time is generally applicable to negative as well as nonnegative operators. However as noted above, when the operator \tilde{V} is negative (i.e., when $|J_+| < \frac{1}{2}$), the intersection of the domains $D(\tilde{T}_\beta) \cap D(\tilde{V})$ is too small to determine a unique self-adjoint extension of \tilde{H} , and the standard Trotter product formula does not apply.

When both \tilde{T}_β and \tilde{V} are nonnegative ($|J_+| \geq \frac{1}{2}$), a result due to Exner et al. (see [5, Theorem 2.2]) allows us to conclude that a version of the Trotter product formula in real time holds with respect to the L^2 norm over time. That is, for nonnegative self-adjoint \tilde{T}_β and \tilde{V} with densely defined form sum $\tilde{T}_\beta + \tilde{V}$ and for any time $T > 0$ and any state $\psi \in L^2(\mathbb{R}^+)$,

$$\lim_{n \rightarrow \infty} \int_{-T}^T \left\| \left(e^{-it\tilde{T}_\beta/\hbar n} e^{-it\tilde{V}/\hbar n} \right)^n \psi - e^{-it(\tilde{T}_\beta + \tilde{V})/\hbar} \psi \right\|_2^2 dt = 0. \quad (6.10)$$

As discussed in [5], this result is weaker than the standard Trotter product formula; however it implies the existence of a subsequence $\{n_k\}$ along which convergence in the strong operator topology holds. This is sufficient to define a time-sliced path integral.

The conditions of the extended Trotter product formula (6.10) are identical to those of the strong Kato–Trotter product formula. Hence an identical analysis determines the self-adjoint extension of \tilde{H} admitting a time-sliced path integral expression. As before, for $|J_+| \geq 1$, $\tilde{T}_0 + \tilde{V}$ coincides with the unique self-adjoint extension of \tilde{H} , while for $\frac{1}{2} < |J_+| < 1$, the restriction (6.3) picks out the $\theta = 0$ extension (Dirichet boundary condition) as that to which (6.10) applies. For $|J_+| = \frac{1}{2}$, the correspondence (6.8) equates $D(\tilde{T}_\beta + \tilde{V})$ to the self-adjoint domain for \tilde{H} with

asymptotics given by (6.7), and each extension admits a Feynman–Kac formula for the real-time evolution operator.

For orderings satisfying $|J_+| \geq 1$ or $|J_+| = \frac{1}{2}$, we have that $D(\tilde{T}_\beta) \cap D(\tilde{V})$ is large enough to determine a unique self-adjoint extension of \tilde{H} , implying that the standard Trotter product formula applies.

6.2.1 Factor orderings with $|J_+| \geq 1$

For factor orderings with $|J_+| \geq 1$, the self-adjoint form sum $\tilde{T}_0 \dot{+} \tilde{V}$ must coincide with the unique self-adjoint extension of \tilde{H} . At the same time, $D(\tilde{T}_0) \cap D(\tilde{V}) \subseteq D(\tilde{T}_0 \dot{+} \tilde{V})$ and $D(\tilde{T}_0) \cap D(\tilde{V})$ is dense (since it contains $C_0^\infty(\mathbb{R}^+)$), so that $\tilde{H} = \tilde{T}_0 \dot{+} \tilde{V}$ is essentially self-adjoint on $D(\tilde{T}_0) \cap D(\tilde{V})$. Thus the standard Trotter product formula applies, and together with the well-known integral kernel [3, 6, 9]

$$g_+^D(t, y, z) = \frac{1}{\sqrt{4\pi it}} [e^{i(y-z)^2/4t} - e^{i(y+z)^2/4t}]$$

for $e^{it\Delta}$ permits a real-time Feynman–Kac formula for $e^{-it\tilde{H}/\hbar}$:

$$\begin{aligned} e^{-it\tilde{H}/\hbar}\psi &= \lim_{n \rightarrow \infty} (e^{-it\tilde{T}_0/\hbar n} e^{-itV(y)/\hbar n})^n \psi = \lim_{n \rightarrow \infty} (e^{iht\Delta/n} e^{-itV(y)/\hbar n})^n \psi \\ &= \lim_{n \rightarrow \infty} \mathcal{N} \int_{\mathbb{R}^+} \cdots \int_{\mathbb{R}^+} \prod_{j=1}^n \left[\left(e^{\frac{in(z_{j+1}-z_j)^2}{4\hbar t}} - e^{\frac{in(z_{j+1}+z_j)^2}{4\hbar t}} \right) e^{\frac{-itV(z_j)}{\hbar n}} \right] \psi(z_1) dz_1 \cdots dz_n, \\ \mathcal{N} &= \left(\frac{n}{4\pi i \hbar t} \right)^{n/2}. \end{aligned} \quad (6.11)$$

As in (6.6), the n -fold measure appearing in (6.11) corresponds to the avoiding measure supported on paths which do not intersect the singularity.

6.2.2 Factor orderings with $\frac{1}{2} < |J_+| < 1$

As discussed above, in this range of orderings the ordinary Trotter product formula does not apply, but the result (6.10) of [5] permits a Feynman–Kac formula. As in the imaginary-time case, the identification of $D(\tilde{T}_\beta \dot{+} \tilde{V})$ with the Dirichlet self-adjoint domain of \tilde{H} ($\theta = 0$), independent of β , implies that without loss of generality, \tilde{T}_0 may be taken as the kinetic term. The Feynman–Kac formula will thus be as in (6.11), with the limit understood to be taken over the subsequence $\{n_k\}$ for which strong operator convergence of the product formula is guaranteed.

6.2.3 Factor orderings with $|J_+| = \frac{1}{2}$

As discussed in the imaginary-time case, for $|J_+| = \frac{1}{2}$ the intersection $D(\tilde{T}_\beta) \cap D(\tilde{V})$ is contained in a unique self-adjoint extension of \tilde{H} , with the correspondence between β and the angle θ of the self-adjoint extension given by (6.8). Since $C_0^\infty(\mathbb{R}^+) \subset D(\tilde{T}_\beta) \cap D(\tilde{V})$ is dense, \tilde{H} is essentially self-adjoint on $D(\tilde{T}_\beta) \cap D(\tilde{V})$ and the standard Trotter product formula again applies.

The integral kernel for $e^{it\Delta}$ with boundary condition $\psi(0) = \beta\psi'(0)$ is given by [3, 6, 9]

$$\begin{aligned} g_+^{(\beta)}(t, y, z) &= \frac{1}{\sqrt{4\pi it}} [e^{i(y-z)^2/4t} + e^{i(y+z)^2/4t}] \\ &\quad - \beta^{-1} \exp \left\{ \frac{it}{\beta^2} + \frac{(y+z)}{\beta} \right\} \operatorname{erfc} \left[\left(\frac{it}{\beta^2} \right)^{1/2} + \left(\frac{y+z}{2\beta} \right) \left(\frac{it}{\beta^2} \right)^{-1/2} \right]. \end{aligned} \quad (6.12)$$

Using (6.12), the time-sliced path integral expression for the real-time evolution operator becomes

$$e^{-it\tilde{H}/\hbar}\psi = \lim_{n \rightarrow \infty} \int_{\mathbb{R}^+} \cdots \int_{\mathbb{R}^+} \prod_{j=1}^n \left[g_+^{(\beta)} \left(\frac{\hbar t}{n}, z_{j+1}, z_j \right) e^{-itV(z_j)/\hbar m} \right] \psi(z_1) dz_1 \cdots dz_n.$$

As with imaginary time, the special cases $\beta = 0$ and $\beta = \infty$ correspond to the Dirichlet and Neumann boundary conditions, with

$$g_+^{(\beta)}(t, y, z) = \begin{cases} \frac{1}{\sqrt{4\pi it}} [e^{i(y-z)^2/4t} - e^{i(y+z)^2/4t}], & \beta = 0, \\ \frac{1}{\sqrt{4\pi it}} [e^{i(y-z)^2/4t} + e^{i(y+z)^2/4t}], & \beta = \infty. \end{cases}$$

The interpretation of the path integral measures as supported on avoiding and reflecting paths for the Dirichlet and Neumann cases, respectively, and of the $\operatorname{erfc}(\cdot)$ term in the integral kernel (6.12) as interpolating between these two cases, remains as in imaginary time.

7 Conclusion

This investigation highlights the effects of factor ordering in circumscribing the range of allowed behaviors for wave functions near the Big Bang/Big Crunch singularity. By generating a sufficiently steep positive quantum potential, orderings with $|J_+| \geq 1$ force the corresponding path integral measure to be supported only on paths which avoid the singularity, while orderings with $|J_+| = \frac{1}{2}$ (including the Laplace–Beltrami/conformal ordering), generating no quantum potential, require an additional boundary condition on wave functions to determine a path integral measure. This boundary condition dictates whether the path integral measure is supported solely on singularity-avoiding paths or whether it has support on paths which reflect off of the singularity.

These results affirm the observation of Kontoleon and Wiltshire [19] regarding the sensitivity of boundary behavior in quantum cosmology to factor ordering. Moreover, the importance of boundary behavior in addressing the question of quantum resolution of the classical Big Bang/Big Crunch singularity has been discussed by Kiefer in [17]; the results in Section 6 reflect the close connection between the support of the path integral measure and the behavior of wave functions near the singularity.

In the sequel we aim to investigate the construction of Hartle–Hawking-type wave functions of the universe using the path integral measures above, and solving the Wheeler–DeWitt equation with corresponding factor ordering. To address the inherent time-reparametrization invariance of (1+1) gravity, it would be of interest to construct time-independent propagators between initial and final states as by Bunster in [33, 34]; in [15], Halliwell implements such methods to yield solutions and Green’s functions for the Wheeler–DeWitt equation in quantum cosmology. Additionally, one could implement the promising methods of Gerhardt in [10] to characterize the space of physical states.

Eventually we expect to broaden the class of factor orderings considered, and ultimately to extend analysis to cosmological models such as Friedmann–Lemaître–Robertson–Walker and Bianchi spacetimes.

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