Calculation of the propagator of Schrödinger’s equation on $(0, \infty)$ with the potential $kx^{2} + \omega^{2}x^{2}$ by Lie symmetry group method

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Abstract
The propagators (fundamental solutions) of the heat and Schrödinger’s equations on the half-line with a combined harmonic oscillator and inverse-square potential calculated in the recent paper [J. Math. Phys. 59, 051507 (2018)] using Laplace’s method are demonstrated to be obtainable alternatively within the framework of symmetry group methods discussed in a series of two papers in the same journal.

Keywords: Green function, linear Schrödinger equation with potential, symmetry group

1 Introduction
Very recently, in Ref. [1], Green function of the operator

$$
P(\partial) = \partial_{t} + \frac{1}{2}(-\partial_{x}^{2} + V(x)) = \partial_{t} - \frac{1}{2}\partial_{x}^{2} + \frac{k}{2}x^{-2} + \frac{1}{2}\omega^{2}x^{2}, \quad k \geq -\frac{1}{4}, \quad \omega \geq 0 \quad (1.1)$$

has been calculated in the half-space $x > 0$ and hence from it that of Schrödinger’s equation with the potential

$$
V(x) = \frac{1}{2}\partial_{x}^{2} + \frac{k}{2}x^{-2} + \frac{1}{2}\omega^{2}x^{2}, \quad k \geq \frac{3}{4}
$$

is deduced using Laplace’s method.
In another recent paper [2] with a reliance on the results of [3], we studied calculation of fundamental solutions of variable coefficient linear parabolic equations allowing sufficiently enough symmetry groups.

The purpose of this paper is to make use of methods from [2, 3] as an alternative natural approach to the one pursued in [1] to derive fundamental solutions for the parabolic operator (1.1) and its Schrödinger variant.

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Two equivalent definitions of fundamental solution

Fundamental solution (the names Green function, source solution, propagator, heat kernel are also used interchangeably) for the initial value problem $u_t - Lu = 0, \ t > 0, \ u(x,0) = f(x), \ x \in \mathbb{R}^n$, where $L = \sum_{|\alpha| \leq m} a_\alpha(x) D^\alpha$, $\alpha \in \mathbb{N}^n$ with the property $a_\alpha \in C^{|\alpha|}(\mathbb{R}^n)$ is a linear differential operator of order $m$, can be defined in two ways.

One way is to define a distribution function $E_\xi(t, x) \in D'(\mathbb{R}^n)$, $t \geq 0$ which solves the following initial value problem

$$(\partial_t - L)E_\xi(t, x) = 0, \ E_\xi(0, x) = \delta(x - \xi), \ x, \xi \in \mathbb{R}^n$$  (2.1)

This is the definition used in Ref. [2].

Another definition is the free space (also called the causal) fundamental solution, which satisfies

$$(\partial_t - L)\tilde{E}_\xi(t, x) = \delta(t)\delta(x - \xi), \ \text{in} \ D'(\mathbb{R}^{n+1}).$$  (2.2)

This definition is used in Ref. [1]. It can be proved that the fundamental solution $E_\xi(t, x)$ as defined in (2.1) coincides with the free-space one when one extends $E_\xi(t, x)$ by zero to $t \leq 0$

$$E_\xi'(t, x) = H(t)E_\xi(t, x) = \begin{cases} E_\xi(t, x), & \text{for} \ t > 0 \\ 0, & \text{for} \ t < 0. \end{cases}$$  (2.3)

The proof that for distributions $E_0(t, x)$ satisfies $(\partial_t - L)E_0'(t, x) = \delta(t, x) = \delta(t)\delta(x)$ can be found in the book [3] for the heat operator, i.e. when $L = \Delta$ is the Laplace operator.

Consequently, all the fundamental solutions constructed here can be easily made to agree with those of Ref. [3] by their extension by zero to $t \leq 0$ just by multiplying them by the Heaviside function $H(t)$ (or $Y(t)$ by the notation of [1]).

3 Calculation of fundamental solution (Green function)

We first consider the operator

$$L = P(\partial) = \partial_t + \frac{1}{2}(-\partial_x^2 + V(x)) = \partial_t - \frac{1}{2}\partial_x^2 + \frac{k}{2}x^{-2} + \frac{1}{2}\omega^2x^2, \ \ k \geq -\frac{1}{4}, \ \ \omega \geq 0$$  (3.1)

and construct the Green function $E_\xi(t, x) \in D'(\mathbb{R}^+)$, $\xi > 0$ in the half-line in the sense of first definition (2.1) for the heat equation with the potential $V(x)$

$$Lu = P(\partial)u = u_t - \frac{1}{2}u_{xx} + \left(\frac{k}{2}x^{-2} + \frac{1}{2}\omega^2x^2\right)u = 0. \quad (3.2)$$
We can get rid of the factors of 1/2 by scaling \( t, t \rightarrow \frac{t}{2} \). We hence consider

\[ u_t = u_{xx} - (kx^{-2} + \omega^2 x^2)u. \]  

(3.3)

A brief summary of the symmetry approach is as follows. We look for a transformation that leaves invariant the initial value problem (2.1) on the half-line \( x > 0 \). Such transformation is realized as a symmetry group of the Lie algebra spanned by the vector fields of the form

\[ \mathbf{v} = \tau(t)\partial_t + \chi(t, x)\partial_x + \phi(t, x)u\partial_u, \]

(3.4)

satisfying the conditions

\[ \tau(0) = 0, \quad \chi(0, \xi) = 0, \quad \phi(0, \xi) + \chi_x(0, \xi) = 0. \]

(3.5)

Fundamental solutions then arise as solutions invariant under this symmetry group. For more details of this and another related method the reader is directed to Ref. [2].

We know from the results of [3] that this equation admits a four-dimensional Lie point symmetry algebra \( \mathfrak{g} \), excluding the obvious infinite-dimensional one, because \( k \neq 0 \) (otherwise 6-dimensional). From the formula (3.28) of Ref. [3] (correcting sign errors in the vector field \( \mathbf{v}_3 \); all signs appearing in the exponentials should be negative) with \( a = 1, b = 0, c = -V(x), I(x) = x, J(x) = 0, c_2 = -\omega^2, c_0 = 0 \) we find the following basis of the symmetry algebra

\[ \mathbf{v}_1 = \partial_t, \]
\[ \mathbf{v}_2 = \cosh(4\omega t)\partial_t + 2\omega \sinh(4\omega t)x\partial_x - [\omega \sinh(4\omega t) + 2\omega^2 \cosh(4\omega t)x^2]u\partial_u, \]
\[ \mathbf{v}_3 = \sinh(4\omega t)\partial_t + 2\omega \cosh(4\omega t)x\partial_x - [\omega \cosh(4\omega t) + 2\omega^2 \sinh(4\omega t)x^2]u\partial_u, \]
\[ \mathbf{v}_4 = u\partial_u \]

(3.6)

with non-zero commutation relations

\[ [\mathbf{v}_1, \mathbf{v}_2] = 4\omega \mathbf{v}_3, \quad [\mathbf{v}_1, \mathbf{v}_3] = 4\omega \mathbf{v}_2, \quad [\mathbf{v}_2, \mathbf{v}_3] = 4\omega \mathbf{v}_1. \]

The general symmetry vector field \( \mathbf{v} = \sum_{i=1}^4 k_i \mathbf{v}_i \) satisfying the initial-boundary conditions \([3, 5]\) is given by

\[ \mathbf{v} = \sinh^2(2\omega t)\partial_t + 2\omega \sinh(4\omega t)x\partial_x + \omega [2\omega x^2 - 2\omega \cosh(4\omega t)x^2 - \sinh(4\omega t)]u\partial_u. \]

(3.7)

We find the invariants of \( \mathbf{v} \) by solving the equation \( \mathbf{v}(\varphi) = 0 \) by the method of characteristics as

\[ \eta = \frac{x}{\sinh(2\omega t)}, \quad \zeta = u^{-1}\sinh(2\omega t)^{-1/2} \exp \left[ -\frac{\omega(x^2 + \xi^2)}{2 \tanh(2\omega t)} \right]. \]

(3.8)

Fundamental solution will be sought as a group-invariant solution in the form

\[ u = \sinh(2\omega t)^{-1/2} \exp \left[ -\frac{\omega(x^2 + \xi^2)}{2 \tanh(2\omega t)} \right] F(\eta). \]

(3.9)
Substitution of (3.9) into (3.3) provides the second order ordinary differential equation (ODE)

\[ \eta^2 F''(\eta) - (\omega^2 \xi^2 \eta^2 + k)F = 0. \]  

(3.10)

The modified Bessel equation of with index \( \nu \) in normal form is

\[ \eta^2 F''(\eta) - (\omega^2 \xi^2 \eta^2 - \frac{1}{4} + \nu^2)F = 0. \]

Hence, the solution of (3.10) bounded near zero can be written as

\[ F = \sqrt{\eta} I_\nu(\omega \xi \eta), \quad \nu = \sqrt{k + \frac{1}{4}} \geq 0, \]

where \( I_\nu \) is the modified Bessel function of the first kind with index \( \nu \). Finally, the fundamental solution \( E_\xi(t, x) \) of (3.2) is determined up to a multiplicative constant \( c_0 \) (after the replacement \( t \to t/2 \))

\[ E_\xi(t, x) = c_0 \frac{\sqrt{x}}{\sinh \omega t} \exp \left[ -\frac{\omega(x^2 + \xi^2)}{2 \tanh(\omega t)} \right] I_\nu \left( \frac{\omega \xi x}{\sinh \omega t} \right). \]  

(3.11)

The constant \( c_0 \) should be found from the normalization condition

\[ \lim_{t \to 0^+} \int_0^\infty E_\xi(t, x) dx = 1. \]

Green function for the special potential when \( \omega = 0 \) has already be obtained in Ref. [2] (page 6) using methods within the symmetry context (with \( k = -\mu \) in notation of [2]). We reproduce it here for the purpose of reference (the replacement \( t \to t/2 \) is done)

\[ E_\xi(t, x) = \frac{\sqrt{\xi x}}{t} \exp \left[ -\frac{x^2 + y^2}{2t} \right] I_\nu \left( \frac{xy}{t} \right), \quad \nu = \sqrt{\frac{1}{4} + k}. \]

We now turn our attention to the construction of Green function for the one-dimensional Schrödinger equation with potential \( V(x) \)

\[ iu_t + u_{xx} = (kx^{-2} + \omega^2 x^2)u, \]  

(3.12)

where \( u : \mathbb{R}_+^2 = \{(t, x) \in \mathbb{R}^2 : x > 0\} \to \mathbb{C} \) is a complex-valued function. From [3], we recall that the symmetry algebra for an arbitrary potential \( V(t, x) \) (with some sign corrections) is represented by

\[ \mathbf{v} = \tau(t) \partial_t + \chi(t, x) \partial_x + i \phi(t, x) u \partial_u, \]

where

\[ \chi(t, x) = \frac{1}{2} \dot{\tau} x + \rho(t), \quad \phi(t, x) = \frac{7}{8} x^2 + \frac{\dot{\rho}}{2} x + \sigma(t) + i \left( \frac{\dot{\tau}}{4} + b \right) \]
and $V$ satisfies the determining equation
\[ \tau V_t + \chi V_x + \dot{\tau} V + \frac{\dot{\tau}}{8} x^2 + \frac{\dot{\rho}}{2} x + \dot{\sigma}(t) = 0. \] (3.13)

Here $b$ is a constant, $\tau(t)$, $\rho(t)$ and $\sigma(t)$ are arbitrary real functions. For the given potential $V = V(x) = kx^{-2} + \omega^2 x^2$, Eq. (3.13) is easily solved for these functions, and it turns out that equation (3.12) admits a five-dimensional symmetry algebra. A basis for its elements is given by
\[
\begin{align*}
\mathbf{v}_1 &= \partial_t, \\
\mathbf{v}_2 &= -\frac{\cos 4\omega t}{4\omega} \partial_t + \frac{\cos 4\omega t}{2} x \partial_x + \frac{1}{4} \left[ 2i\omega \cos(4\omega t)x^2 - \sin 4\omega t \right] u \partial_u, \\
\mathbf{v}_3 &= \frac{\sin 4\omega t}{4\omega} \partial_t + \frac{\sin 4\omega t}{2} x \partial_x - \frac{1}{4} \left[ 2i\omega \sin(4\omega t)x^2 + \cos 4\omega t \right] u \partial_u, \\
\mathbf{v}_4 &= u \partial_u + u^* \partial_{u^*}, \\
\mathbf{v}_5 &= i(u \partial_u - u^* \partial_{u^*}),
\end{align*}
\] (3.14)

where $^*$ denotes the complex conjugation and in $\mathbf{v}_2$ and $\mathbf{v}_3$ complex conjugated coefficients of $u$-component are omitted. Again, the most general symmetry element leaving the initial condition $\lim_{t \to 0} E_\xi(t, x) = \delta(x - \xi)$ invariant has the form
\[
\mathbf{v} = 2 \sin^2(2\omega t) \partial_t + 2\omega \sin(4\omega t)x \partial_x + i\omega \left[ -2\omega \xi^2 + 2\omega \cos(4\omega t)x^2 + i\sin(4\omega t) \right] u \partial_u.
\] (3.15)

Invariants are $\eta = x / \sin(2\omega t)$ and $\zeta = u^{-1}(\sin 2\omega t)^{-1/2} \exp[2^{-1}i\omega(x^2 + \omega^2) \cot(2\omega t)]$. Green function will be of the form
\[
u = (\sin 2\omega t)^{-1/2} \exp \left[ \frac{i\omega(x^2 + \omega^2)}{2 \tan(2\omega t)} \right] F(\eta).
\] (3.16)

When substituted into (3.12) we find that $F$ should satisfy the ODE
\[
\eta^2 F''(\eta) + (\omega^2 \xi^2 \eta^2 - k) F(\eta) = 0.
\] (3.17)

which is the normal form of the Bessel equation with index $\nu = \sqrt{\frac{1}{4} + k}$. Therefore, the Green function of Eq. (3.12), up to a nonzero normalization constant, is given by
\[
E_\xi(t, x) = c_0 \sqrt{x / \sin \omega t} \exp \left[ \frac{i\omega(x^2 + \xi^2)}{2 \tan(\omega t)} \right] J_\nu \left( \frac{\omega \xi x}{\sin \omega t} \right).
\] (3.18)

The calculation of the Green function of (3.12) for $\omega = 0$ is slightly different in which the relevant symmetry vector field now becomes a projective type
\[
\mathbf{v} = t^2 \partial_t + x t \partial_x + \frac{1}{4} \left[ i(x^2 - \xi^2) - 2t \right] u \partial_u.
\] (3.19)

In this situation, solution ansatz (using invariants of $\mathbf{v}$) will be in the form
\[
u = \frac{1}{\sqrt{t}} \exp \left[ \frac{i(x^2 + \xi^2)}{4t} \right] F(\eta), \quad \eta = \frac{x}{t},
\] (3.20)
where the function $F$ satisfies

$$\eta^2 F''(\eta) + \left( \frac{\xi^2}{4} \eta^2 - k \right) F(\eta) = 0 \quad (3.21)$$

with the appropriate solution $F = \sqrt{\eta} J_\nu(\frac{\xi \eta}{2}), \nu = \sqrt{\frac{1}{4} + k}$. Finally, the Green function (up to a normalization constant) is given by

$$E_\xi(t, x) = c_0 \sqrt{\frac{x}{t}} \exp\left[ \frac{i(x^2 + \xi^2)}{4t} \right] J_\nu(\frac{\xi x}{t}). \quad (3.22)$$

$E_\xi(t, x)$ given in $(3.18)$ and $(3.22)$ is smooth if $x \neq 0$, $(t, x) \neq (0, \xi)$, namely of class $C^\infty(\mathbb{R} \times \mathbb{R}^n \setminus (0, \xi))$ (See [1] for their remarkable properties).

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