Line Laplace Transforms for obtaining the Exact Bound States for the Morse Potential

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Abstract
The line Laplace transforms is applied to the Morse potential. The wavefunctions and the energy levels through suitable path of integration are derived.
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1 Introduction
The Morse potential [1] is one of the simplest example of the Natanzon potentials [2] which has a finite number of the bound–states. It was introduced by P. M. Morse in 1929 as a model to describing the vibrational energy of a diatomic molecule and takes the form
\[ V(x) = V_0 \left(1 - e^{-ax}\right)^2, \] (1)
where \( x \) represents a bond length, \( a \) a parameter controlling the potential width, and \( V_0 \) the dissociation energy of the molecule.

Several authors have investigated the exact solvability of Schrödinger equation with the Morse potential using various approaches and numerous papers have been increased in recent years, dealing with supersymmetric quantum mechanics [3,4,5], \textit{so} (2,1) and \textit{su} (1,1) Lie algebras [6,7,8,9], the point canonical transformations [10], variational method [11], path–integral approach [12], coherent states [13] and recently the Nikiforov–Uvarov method [14], are used in order to provide the exact solution of the eigenfunctions and corresponding energy eigenvalues for the Morse potential. It is also well known that the Morse potential have a causal connection with the Pöschl–Teller potential [15] and Coulomb potential [16].

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Perhaps the most useful integral transforms frequently used in mathematical physics and physical applications is Laplace transforms [17,18]. The main application of the Laplace transforms consists probably in converting differential equation into simpler forms that may be solved easily [19,20].

In the present paper, we will perform the line Laplace transforms to solve the Schrödinger equation with the Morse potential. We investigate how the mathematical formalism of this method works to deduce the wavefunctions and energy levels for the Morse potential. This simply means that the choice of the path of integration \( l \) must be specified. We will see that unless the integrand has special properties, that lead the wavefunction integral to depend only on the value of the end points; the value will depend on the particular choice of the contour \( l \).

This work is organized as follows: in the second section we perform the line Laplace transforms in order to deal with the Morse potential. Section three is devoted to obtaining the exact bound–states for the Morse potential by choosing a suitable path of integration and in the last section we do our final conclusion.

## 2 Condition on the wavefunction \( F (\xi) \)

Following [19] and [20], the Schrödinger equation of the Morse potential (1) is given by

\[
\left[ \frac{d^2}{dx^2} - \frac{2mV_0}{\hbar^2} e^{-2ax} + \frac{4mV_0}{\hbar^2} e^{-ax} + \frac{2m}{\hbar^2} (E - V_0) \right] \psi(x) = 0.
\] \( (2) \)

Introducing the new change of variable and new wavefunction as

\[
\xi = k e^{-ax}, \quad \text{with} \quad k = \frac{2\sqrt{2mV_0}}{\alpha \hbar}, \quad (3.a)
\]

\[
\psi(x) = \xi^\mu F(\xi), \quad (3.b)
\]

where \( \xi \in [0, \infty] \) and \( \mu \) is a constant, allow to transforming Eq.(2) into

\[
\left[ \xi^2 \frac{d^2}{d\xi^2} + (2\mu + 1) \frac{d}{d\xi} - \frac{k}{4} \xi^2 + \frac{k}{2} \xi + \mu^2 - \beta^2 \right] F(\xi) = 0, \quad (4)
\]

where \( \beta = \sqrt{-\frac{2m}{\alpha^2 \hbar^2} (E - V_0)} \). Putting \( \mu = -\beta \) [19,20], we get the differential equation

\[
\left[ \xi^2 \frac{d^2}{d\xi^2} - (2\beta - 1) \frac{d}{d\xi} - \frac{1}{4} \xi + \frac{k}{2} \right] F(\xi) = 0, \quad (5)
\]

where Eq.(5) accepts a regular point at \( \xi = 0 \) and an irregular one at \( \xi = \infty \).

Let us consider the function \( F(\xi) \) can be expressed as an integral of the general form

\[
F(\xi) = \int_l f(t) e^{\xi t} dt, \quad (6)
\]

where \( f(t) \) is an unknown function and \( l \) is the path of integration which does not depend on \( \xi \). The integral (6) is often called the line Laplace transforms.
Then, by applying the derivative of $F(\xi)$ with respect to $\xi$, one obtains

\[ F'(\xi) = \oint_l t f(t) e^{\xi t} dt, \quad \text{(7.a)} \]

\[ F''(\xi) = \oint_l t^2 f(t) e^{\xi t} dt. \quad \text{(7.b)} \]

Multiplying Eqs.(6) and (7.b) by $\xi$ and performing derivation by parts, we get

\[ \xi F(\xi) = \{f(t) e^{\xi t}\}_l - \oint_l \frac{df(t)}{dt} e^{\xi t} dt, \quad \text{(8.a)} \]

\[ \xi F''(\xi) = \{t^2 f(t) e^{\xi t}\}_l - \oint_l \frac{d[t^2 f(t)]}{dt} e^{\xi t} dt, \quad \text{(8.b)} \]

where the symbol $\{Y(t)\}_l$ denotes the increase of $Y(t)$ when $t$ describes the contour $l$.

Substituting Eqs.(6), (7.a) and (8.b) into the differential equation (5), we obtain

\[ \left[ f(t) \left( t^2 - \frac{1}{4} \right) e^{\xi t} \right]_l - \oint_l \left\{ \frac{d[t^2 f(t)]}{dt} - \frac{1}{4} \frac{df(t)}{dt} + \left( 2\beta - 1 \right) t - \frac{k}{2} \right\} f(t) e^{\xi t} dt = 0. \quad \text{(9)} \]

The contour of integration $l$ is then chosen so that the first term in Eq.(9) vanishes and that the integrand will vanish at the end points; these considerations lead to write

\[ \frac{d[t^2 f(t)]}{dt} - \frac{1}{4} \frac{df(t)}{dt} + \left( 2\beta - 1 \right) t - \frac{k}{2} f(t) = 0. \quad \text{(10)} \]

Taking into account the differentiation of Eq.(10) and integrating the result, we get

\[ f(t) = C_{p,q} \left( t - \frac{1}{2} \right)^{p-1} \left( t + \frac{1}{2} \right)^{q-1}, \quad \text{(11)} \]

where $C_{p,q}$ is a constant of integration and the parameters $p$ and $q$ are defined as

\[ p - 1 = \frac{k}{2} - \frac{2\beta + 1}{2}, \quad q - 1 = -\frac{k}{2} - \frac{2\beta + 1}{2}, \quad \text{(12)} \]

and then the integral (6) may be written

\[ F(\xi) = C_{p,q} \oint_l \left( t - \frac{1}{2} \right)^{p-1} \left( t + \frac{1}{2} \right)^{q-1} e^{\xi t} dt, \quad \text{(13)} \]

is a solution of differential equation (5) and the contour, by virtue of the condition quoted above, must verify

\[ \left\{ \left( t - \frac{1}{2} \right)^p \left( t + \frac{1}{2} \right)^q e^{\xi t} \right\}_l \equiv 0. \quad \text{(14)} \]
3 Wavefunctions and energy levels

From Eq.(12), the parameters $p$ and $q$ are not integer and defined positive\footnote{We verify this assumption below; cf. relationship (19.a–b).}, then the integrand in (13) has a branch points at $t_{\pm} = \pm \frac{1}{2}$ [17], and the product $(t - \frac{1}{2})^p (t + \frac{1}{2})^q$ in Eq.(14) will vanish for $t_{\pm}$. The integrand into (13) is therefore single–Valued for the contour encircling both branch points; i.e. taking the line segment joining $t_+ = \frac{1}{2}$ and $t_- = -\frac{1}{2}$ as a cut line [17].

Let us consider a particular choice of the contour such as

$$l = \left\{ t \in \left[-\frac{1}{2}, \frac{1}{2}\right] \mid s = \xi \left(t + \frac{1}{2}\right) \right\},$$

therefore Eq.(13) becomes

$$F(\xi) = (-1)^{p-1} C_{p,q} e^{-\xi/2} \xi^{1-p-q} \int_{0}^{\xi} s^{q-1} (\xi - s)^{p-1} e^s ds. \tag{16}$$

Using the integral representation [21, cf. 9.211 2, pp. 1058]

$$1F_1 (\alpha; \gamma; \xi) = \frac{1}{B (\alpha, \gamma - \alpha)} \xi^{1-\gamma} \int_{0}^{\xi} s^{\alpha-1} (\xi - s)^{\gamma-\alpha-1} e^s ds, \quad \text{[Re } \gamma > \text{Re } \alpha > 0], \tag{17}$$

the integral into Eq.(16) becomes

$$\int_{0}^{\xi} s^{q-1} (\xi - s)^{p-1} e^s ds = B (q, p) \ 1F_1 (1 - p; 2 - p - q; \xi), \tag{18}$$

where $1F_1 (\alpha; \gamma; \xi)$ is the confluent hypergeometric function and $B (\alpha, \gamma - \alpha) = \frac{\Gamma(\alpha)\Gamma(\gamma - \alpha)}{\Gamma(\gamma)}$ is the beta function [17], with $p+q = \gamma$ and $\alpha = q$. In terms of Eqs.(12), the parameters in Eq.(18) read

$$1 - p \equiv 1 + \alpha - \gamma = -\frac{k}{2} + \frac{2\beta + 1}{2}, \tag{19.a}$$

$$2 - p - q \equiv 2 - \gamma = 2\beta + 1. \tag{19.b}$$

Then, the function $F(\xi)$ reads as

$$F(\xi) = \mathcal{N}_{p,q} e^{-\xi/2} \xi^{1-p-q} 1F_1 (1 - p; 2 - p - q; \xi), \tag{20}$$

where $\mathcal{N}_{p,q} = (-1)^{1-p} C_{p,q} B (q, p)$.

However, it is well known that the (confluent) hypergeometric function becomes a simple polynomial if and only if the parameter $1 - p$ in Eq.(20) equals 0 or a negative integer [17]. We limit ourselves here to second case, i.e. $1 - p = -n$, leading to identify

$$k - (2\beta + 1) = 2n, \tag{21}$$
where \( n \) is called the vibrational quantum number and takes the values \( n = 0, 1, 2, \ldots n_{\text{max}} \). Substituting Eqs. (19.a–b) and (21) into Eq. (20), and the result into Eq. (3.b), the wavefunction \( \psi (\xi) \) is then given by

\[
\psi (\xi) = \xi^\mu F (\xi) = N_{p,q}^{(n)} e^{-\xi/2} \xi^\beta \, _1F_1 (-n; 2\beta + 1; \xi). \tag{22}
\]

Inserting the parameters \( \beta \) and \( k \) as defined hereabove into Eq. (21), then the corresponding energy levels are

\[
E_n = -V_0 \left[ 1 - \frac{ah}{\sqrt{2mV_0}} \left( n + \frac{1}{2} \right) \right]^2 + V_0. \tag{23}
\]

and which Eqs. (22) and (23) agree with those obtained by [19,20].

4 Conclusion

We investigated a simple method of line Laplace transforms of finding the wavefunctions and the corresponding energy levels of the Schrödinger equation with the Morse potential. The approach developed here has not brought anything new, however, the main purpose is to investigate how the method of line Laplace transforms works. We have shown that applying the specific choice of the contour \( l \), we can find one of the various integral representations of the confluent hypergeometric functions and which are associated with wavefunctions of the Morse potential.

Since there are other closely integral representations of confluent hypergeometric functions, we attempt that they can be other contours of integration used to get the wavefunctions of the Morse potential.

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