Path Integral Solution of PT-/non-PT-Symmetric and non-Hermitian Morse Potential

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Abstract

Path integral solutions are obtained for the the PT-/non-PT-Symmetric and non-Hermitian Morse Potential. Energy eigenvalues and the corresponding wave functions are obtained.

Keywords: PT-symmetry, coherent states, path integral, Morse potential

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I. INTRODUCTION

The concept of PT-symmetry has received much interest in recent years in one dimensional solutions of some quantum mechanical problems. In the standard axiom of quantum mechanics, to have a real energy spectrum, Hamiltonian must be hermitian: \( H = H^\dagger \). In the PT-symmetric quantum mechanics which is an alternative to standard axiom case, Hamiltonian has real spectrum although it is not Hermitian. When PT-symmetry is not spontaneously broken, PT-symmetric and non hermitian complex potentials have a real energy spectrum \[1\]. If any potential under the transformations \( x \rightarrow -x \) (or \( x \rightarrow \xi - x \)) and \( i \rightarrow -i \), satisfies \( V(-x) = V^*(-x) \), it is said to be PT-symmetric. PT-symmetric and non-Hermitian Hamiltonians having real and/or complex eigenvalues are calculated energy spectrum and corresponding wave functions numerically and analytically \[4, 5\].

In this work, Feynman’s path integral method is used in order to get energy spectrum and wave functions of PT-/non-PT-Symmetric and non-Hermitian Morse Potential \[14, 15\] which is exactly solvable \[2, 10\]. The potentials are solved reducing to quadratic forms with a parametric time transformation and a canonical point transformation. The Morse potential is used to describe interaction of the atoms in the diatomic molecules. \[17\]. The generalized Morse potential is

\[
V(x) = V_1 e^{-2\alpha(r-r_0)} - V_2 e^{-\alpha(r-r_0)}. \tag{1}
\]

where \( r \) is the internuclear distance between the two atoms, \( r_0 \) is location of the potential minimum and \( V_1, V_2 \) parameters are functions determined well depth.

The paper is organized as follows: In section II, we introduce the calculation of the energy eigenvalues and the corresponding wave functions of Generalized Morse Potential by using Path integral method. In section III and IV, solutions of PT-/non-PT-symmetric and non Hermitian forms of the generalized Morse potentials are presented by using Path integral method. We summarize the conclusions in section V.

II. GENERALIZED MORSE POTENTIAL

We use path integral technique developed by Duru and Kleinert \[2\] to calculate the energy eigenvalues and the corresponding wave function of PT-/non-PT-Symmetric and
non-Hermitian generalized Morse Potential. The kernel is defined by the usual phase space path integral in cartesian coordinates:

\[
K(x_b, t_b; x_a, t_a) = \int \frac{DxDt}{2\pi} e^{\exp\{i \int dt[p\dot{x} - \frac{p^2}{2m} - V(x)]\}}
\]  

(\hbar = 1). This is the probability amplitude of a particle traveling from a position \(x_a\) at time \(t_a\) to \(x_b\) at time \(t_b\). The time interval can be divided into \(n\)-equal parts. Thus one can get

\[
t_j - t_{j-1} = t_b - t_a = T \quad j = 1, 2, 3...N
\]  

and

\[
x_j = x(t_j), \quad x_0 = x_a, \quad x_N = x_b.
\]  

The kernel can be rewritten as the limiting case of the usual time graded form

\[
K(x_b, T; x_a, 0) = \int_{-\infty}^{\infty} \prod_{i=1}^{n} dx_i \prod_{j=1}^{n+1} dp_i \frac{2\pi}{2\pi} e^{\exp\{i \sum_{j=1}^{n+1} [p_i(x_i - x_{i-1}) - \frac{p_i^2}{2m} - V(x_i)]\}}
\]  

or

\[
K(x_b, T; x_a, 0) = \int_{-\infty}^{\infty} \prod_{j=1}^{n} dx_j \prod_{j=1}^{n+1} dp_j \frac{2\pi}{2\pi} e^{\exp\{i \sum_{j=1}^{n+1} [p_j(x_j - x_{j+1}) - \frac{p_j^2}{2m} - V(x_j)]\}}.
\]  

These forms are the same, since in the application of the point transformation, \(dp_0\) integration comes in the use of Eq. (6) while a \(dp_{n+1}\) momentum integration comes in the Eq. (5) case. We apply the point transformation by using Eq. (5). To have a solvable path integral form for the generalized Morse potential, we define

\[
e^{-\alpha x} = u^2 \quad p_x = -\frac{\alpha u}{2} p_u.
\]  

Thus, the contribution to Jacobien becomes

\[
\frac{DxDp}{2\pi} = -\frac{\alpha}{2u_b} \frac{DuDp_u}{2\pi}
\]  

and the transformed kernel takes

\[
K(x_b, T; x_a, 0) = -\frac{\alpha}{2u_b} \int \frac{DuDp_u}{2\pi} e^{\exp[i \int dt(p_u\dot{u} - \frac{u^2}{2(4m/\alpha^2)} p_u^2 - V_1 u^4 + V_2 u^2)]}.
\]
To eliminate the \( \dot{u}^2 \) term in the kinetic energy part, we introduce a new time parameter \( s \) [2, 10], such that

\[
\frac{dt}{ds} = \frac{1}{u^2} \quad \text{or} \quad t = \int \frac{ds'}{u^2(s')}. \tag{10}
\]

Using Fourier expression of \( \delta \)–function and \( S = s_b - s_a \), parametric time definition can be written as

\[
1 = \int dS \frac{1}{u_b} \delta(T - \int \frac{ds}{u^2}) = \int dS \int \frac{dE}{2\pi u_b^2} \exp[i(ET - \int ds \frac{E}{u^2})]. \tag{11}
\]

Therefore Eq. (9) becomes

\[
K(x_b, T; x_a, 0) = \frac{\alpha}{2} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{iET} \int_0^\infty dS e^{iV_s} \int \frac{1}{u_b} \frac{Du Dp_a}{2\pi} \exp[i \int_0^S ds (p_a \dot{u} - \frac{p_a^2}{2M} - \frac{1}{2} M \omega^2 u^2 - \frac{E}{u^2})] \tag{12}
\]

where

\[
M = \frac{4m}{\alpha^2}, \quad \omega = \sqrt{\frac{V_1}{M}}. \tag{13}
\]

Eq. (12) can be rewritten as

\[
K(x_b, T; x_a, 0) = \frac{\alpha}{2} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{iET} \int_0^\infty dS e^{iV_s} K(u_b, S; u_a, 0). \tag{14}
\]

If we integrate over \( Dp_a \), we get

\[
K(u_b, S; u_a, 0) = \int \frac{1}{u_b} Du \exp[i \int_0^S ds (\frac{1}{2} M \dot{u}^2 - \frac{1}{2} M \omega^2 u^2 - \frac{E}{u^2})]. \tag{15}
\]

The factor \( \frac{1}{u_b} \) here is the result of \( \delta \)-function normalization and transformation in Eq. (8). It appears in the use of Eq. (6). To symmetrize it, we write as

\[
\frac{1}{u_b} = \frac{1}{(u_a u_b)^{1/2}} \exp(-\frac{1}{2} \ln \frac{u_b}{u_a}) = \frac{1}{\sqrt{u_a u_b}} \exp(-\frac{1}{2} \int_0^S ds \frac{\dot{u}}{u}) = \frac{1}{\sqrt{u_a u_b}} \exp[i \int_0^S ds \frac{\dot{u}}{2u}]. \tag{16}
\]

Therefore Eq. (14) can be written
\[ K(u_b, S; u_a, 0) = \frac{1}{\sqrt{u_a u_b}} \int \frac{Dp_a}{2\pi} \]
\[ \times \exp[i \int_0^S ds \left(p_a \dot{u} - \frac{p_a^2}{2M} - \frac{1}{2} M \omega^2 u^2 - \frac{2ME - 1/4}{2Mu^2} + \frac{ip_a}{2Mu}\right)]. \quad (17) \]

Symmetrizing the factor \( \frac{1}{u_a} \) in the same way, we get
\[ \frac{1}{u_a} = \frac{1}{\sqrt{u_a u_b}} \exp[-i \int_0^S ds \frac{i \dddot{u}}{2u}] \quad (18) \]
and kernel can be written as
\[ K(u_b, S; u_a, 0) = \frac{1}{\sqrt{u_a u_b}} \int \frac{Dp_a}{2\pi} \]
\[ \times \exp[i \int_0^S ds \left(p_a \dot{u} - \frac{p_a^2}{2M} - \frac{1}{2} M \omega^2 u^2 - \frac{2ME - 1/4}{2Mu^2} + \frac{ip_a}{2Mu}\right)]. \quad (19) \]

Quantum mechanical contribution to the kernel in Eq. (17) is \( \frac{1}{8M \omega^2} + \frac{ip_a}{2Mu} \). While this term in Eq. (19) is due to Jacobien’s symmetry. Since the kernels in Eqs. (5) and (6) are equivalent. Eq. (17) and Eq. (19) must be equivalent. Thus using geometric average, we obtain
\[ \overline{K}(u_b, S; u_a, 0) = \frac{1}{\sqrt{u_a u_b}} \int \frac{Dp_a}{2\pi} \exp\left\{i \int_0^S ds \left[p_a \dot{u} - \frac{p_a^2}{2M} - \frac{1}{2} M \omega^2 u^2 - \frac{2ME - 1/4}{2Mu^2}\right]\right\}. \quad (20) \]

It has an effective Hamiltonian as seen
\[ H_{eff} = \frac{p_a^2}{2M} + \frac{1}{2} M \omega^2 u^2 + \frac{2ME - 1/4}{2Mu^2}. \quad (21) \]

So the problem
\[ V(u(s)) = \frac{1}{2} M \omega^2 u^2 + \frac{2ME - 1/4}{2Mu^2} \quad (22) \]
is taken as the new potential of the moving particle. Thus we see that the solution is reduced to harmonic oscillator case in polar coordinates [8]. \( \overline{K}(u_b, S; u_a, 0) \) can be obtained as
\[
\mathcal{K}(u_b, S; u_a, 0) = \frac{M\omega\sqrt{u_au_b}}{i\sin \omega S} \exp \left[ iM\omega \left( u_a^2 + u_b^2 \right) \cot \omega S \right] I_{\sqrt{2ME}} \left( \frac{M\omega u_a u_b}{i\sin \omega S} \right).
\]

(23)

The energy eigenvalues and wave functions for generalized Morse potential can be calculated by using Eq. (23). For this, we use the Hille-Hardy formula [21]

\[
t e^{-\alpha/2} \frac{1}{1-t} \exp \left[ -\frac{1}{2} (x+y) \frac{1+t}{1-t} \right] I_{\alpha} \left( \frac{2\sqrt{xy(t+1)}}{t} \right) = \sum_{n=0}^{\infty} \frac{t^n n! e^{-\frac{1}{2}(x+y)}}{\Gamma(n+\alpha+1)} (xy)^{\frac{\alpha}{2}} L_n^{(\alpha)}(x)L_n^{(\alpha)}(y).
\]

(24)

Substituting \( t = e^{-2i\omega S} \), \( x = M\omega u_a^2 \) and \( y = M\omega u_b^2 \) in Eq. (23), we can write Eq. (23) as

\[
\mathcal{K}(u_b, S; u_a, 0) = \sum_{n=0}^{\infty} e^{i\epsilon_n S} \psi_n(u_b)\psi^*_n(u_a)
\]

(25)

where the energy \( \epsilon_n \) is given by

\[
\epsilon_n = \omega \left( 2n + 1 + \sqrt{2ME} \right).
\]

(26)

From Eq. (24) wave functions are obtained as

\[
\psi_n(u) = \sqrt{\frac{2M\omega n! \Gamma(n + 2s + \frac{1}{2})}{u_n!}} (M\omega u^2)^{s+\frac{1}{2}} \exp \left( -M\omega u^2 \right) L_n^{2s+\frac{1}{2}} (M\omega u^2).
\]

(27)

Here \( s = \frac{1}{4} + \frac{1}{2}\sqrt{2mE} > 0 \), \( n = 0, 1, 2... \) and \( L_n^{2s+\frac{1}{2}} (M\omega u^2) \) is associated Laguerre polynomials. Therefore we calculate the energy dependent Greens function for the generalized Morse potential

\[
G(u_b, u_a; E) = -\frac{\alpha}{2\sqrt{u_a u_b}} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{iET} \sum_{n=0}^{\infty} \int_{0}^{\infty} dS e^{(iv_2 - \epsilon_n)S} \psi_n(u_b)\psi^*_n(u_a)
\]

\[
= \sum_{n=0}^{\infty} \exp \left\{ -i \left[ -v_2 \left( 1 - \frac{2\omega}{V_2} \left( n + \frac{1}{2} \right) \right)^2 \right] T \right\} \phi_n(u_b)\phi^*_n(u_a).
\]

(28)

Integrating over \( dS \) and \( dE \), we can get energy eigenvalues

\[
E_n = -v_2 \left[ 1 - \frac{2\omega}{V_2} \left( n + \frac{1}{2} \right) \right]^2, \quad n = 0, 1, 2... < \frac{V_2}{\omega} - \frac{1}{2}
\]

(29)
and normalized wave functions are

\[ \phi_n(u) = \sqrt{\frac{2\alpha(s - \frac{1}{4})M\omega^n!}{\Gamma(n + 2s + \frac{1}{2})}} (M\omega u^2)^{s + \frac{1}{2}} \exp(-M\omega u^2) L_{n}^{2s + \frac{1}{2}} (M\omega u^2) \]  

Therefore, PT-symmetric and Hermitian generalized Morse potential have these wave functions and energy eigenvalues.

III. PT-SYMMETRIC AND NON-HERMITIAN MORSE POTENTIAL CASE

If \( V_1 \) and \( V_2 \) are real and \( \alpha = i\alpha \) then the Morse potential has the form

\[ V(x) = V_1 e^{-2i\alpha x} - V_2 e^{-i\alpha x}. \]  

We can get wave functions and energy eigenvalues following the same steps. This time, we use a coordinate transformation \( u(t) = e^{-i\alpha x} \) and a new time parameter \( s \) defined as

\[ \frac{dt}{ds} = -\frac{1}{u^2}. \]  

Thus the kernel becomes

\[ K(x_b, T; x_a, 0) = -\frac{i\alpha}{2} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{iET} \int_{0}^{\infty} dS e^{-iV_2 S} \int \left( \frac{1}{u_b} \right) \frac{DuDP_u}{2\pi} \times \exp \left[ i \int_{0}^{S} ds (p_u \dot{u} - \frac{p_u^2}{2M} - \frac{1}{2} M\omega^2 u^2 + E) \right] \]  

where

\[ M = \frac{4m}{\alpha^2}, \quad \omega = \sqrt{-\frac{V_1}{M}}. \]  

Frequency is defined as \( \omega = \sqrt{-\frac{V_1}{M}} \) and energy is \( V_2 \). Applying the symmetrization of Jacobien in the same way, kernel takes
\[ K(u_b, S; u_a, 0) = \frac{1}{\sqrt{u_a u_b}} \int \frac{Du Dp_u}{2\pi} \exp \left\{ i \int_0^S ds [p_u \dot{u} - \frac{p_u^2}{2M} - \frac{1}{2} M \omega^2 u^2 - \left( \frac{\sqrt{-2M E}}{2M} \right)^2 - 1/4] \right\}. \]  

(35)

So, effective Hamiltonian of the system is written as

\[ H_{\text{eff}} = \frac{p_u^2}{2M} + \frac{1}{2} M \omega^2 + \left( \frac{\sqrt{-2M E}}{2M} \right)^2 - 1/4. \]  

(36)

Applying the same procedure, kernel can be obtained as

\[ K(u_b, S; u_a, 0) = \frac{M \omega}{i \sin \omega S} \exp \left[ \frac{i M \omega}{2} (u_a^2 + u_b^2) \cot \omega S \right] I \sqrt{-2M E} \left( \frac{M u_a u_b}{i \sin \omega S} \right). \]  

(37)

Therefore, Greens function becomes

\[ G(u_b, u_a; E) = -\frac{i \alpha}{2\sqrt{u_a u_b}} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{i ET} \sum_{n=0}^{\infty} \int_0^\infty dS e^{(-iV_2 - \varepsilon_n)S} \psi_n(u_b) \psi^*_n(u_a) \]

\[ = \sum_{n=0}^{\infty} \exp \left\{ -i \left[ V_2 \left( 1 + \frac{2\omega}{V_2} (n + \frac{1}{2}) \right)^2 \right] T \right\} \phi_n(u_b) \phi^*_n(u_a). \]  

(38)

Energy eigenvalues are

\[ E_n = -V_2 \left[ 1 + \frac{2\omega}{V_2} (n + \frac{1}{2}) \right]^2, \quad n = 0, 1, 2, \ldots < \frac{V_2}{\omega} + \frac{1}{2} \]  

(39)

and normalized wave functions become

\[ \phi_n(u) = \sqrt{\frac{2\alpha(s - \frac{1}{4})M \omega n!}{\Gamma(n + 2s + \frac{1}{2})}} (M \omega u^2)^{s + \frac{1}{2}} \exp \left( -M \omega u^2 \right) L_n^{2s + \frac{1}{2}} (M \omega u^2), \]  

(40)

where \( s = \frac{1}{2} + \frac{1}{2}\sqrt{-2mE}, \quad n = 0, 1, 2, \ldots \)

IV. NON-PT-SYMMETRIC AND NON-HERMITIAN MORSE POTENTIAL CASE

If we take \( V_1 = (A + iB)^2, \) \( V_2 = (2C + 1)(A + iB) \) and \( \alpha = 1, \) the Morse potential takes

\[ V(x) = (A + iB)^2 e^{-2x} - (2C + 1)(A + iB) e^{-x}. \]  

(41)
Here $A, B, C$ are arbitrary parameters. This potential is non-PT symmetric and non-Hermitian, but has real spectra. If $V_1$ is real $V_2 = A + iB$ and $\alpha = i\alpha$ the Morse potential has the form

$$V(x) = V_1 e^{-2i\alpha x} - (A + iB) e^{-i\alpha x}. \quad (42)$$

We can derive wave functions and energy eigenvalues in the same way. This time, we use a coordinate transformation $u(t) = e^{-i\alpha x}$ and define a new time parameter, then the kernel becomes

$$K(x_b; T; x_a, 0) = \frac{i\alpha}{2} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{iET} \int_{-\infty}^{\infty} dS e^{-i(A+iB)S} \int \left( \frac{1}{u_b} \frac{DuDp_a}{2\pi} \right) \exp\left[ i \int_0^S ds(p_a\dot{u} - \frac{p_a^2}{2M} - \frac{1}{2} M\omega^2 u^2 + E \frac{u}{u^2}) \right]$$

$$\times \exp\left[ i \int_0^S ds(p_a\dot{u} - \frac{p_a^2}{2M} - \frac{1}{2} M\omega^2 u^2 + E \frac{u}{u^2}) \right] \quad (43)$$

where

$$M = \frac{4m}{\alpha^2}, \quad \omega = \sqrt{-\frac{V_1}{M}} \quad (44)$$

Frequency is defined as $\omega = \sqrt{-\frac{V_1}{M}}$ and energy is $(A + iB)$. Applying the symmetrization of Jacobien in the same way, kernel becomes

$$K(u_b; S; u_a, 0) = \frac{1}{\sqrt{u_a u_b}} \int \frac{DuDp_a}{2\pi} \exp\left\{ i \int_0^S ds[p_a\dot{u} - \frac{p_a^2}{2M} - \frac{1}{2} M\omega^2 u^2 - \left( \frac{-2ME}{2Mu^2} \right)^2 - 1/4] \right\}. \quad (45)$$

So, effective Hamiltonian of the system is written as

$$H_{eff} = \frac{p_a^2}{2M} + \frac{1}{2} M\omega^2 + \frac{\left( \frac{-2ME}{2Mu^2} \right)^2 - 1/4}{2Mu^2}. \quad (46)$$

Applying the same procedure, kernel can be obtained as

$$K(u_b; S; u_a, 0) = \frac{M \omega \sqrt{u_a u_b}}{i \sin \omega S} \exp\left[ i \frac{M \omega}{2} (u_a^2 + u_b^2) \cot \omega S \right] I_{\sqrt{-2ME}} \left( \frac{M \omega u_a u_b}{i \sin \omega S} \right). \quad (47)$$

Therefore, Greens function becomes
\[ G(u_b, u_a; E) = -\frac{i\alpha}{2\sqrt{u_a u_b}} \int_{-\infty}^{\infty} dE e^{iET} \sum_{n=0}^{\infty} \int_0^{\infty} dS e^{-i(A+iB-\epsilon_n)S} \psi_n(u_b)\psi_n^*(u_a). \] (48)

Energy eigenvalues are

\[ E_n = -(A + iB) \left[ 1 + \frac{2\omega}{A + iB}(n + \frac{1}{2}) \right]^2, \quad n = 0, 1, 2, ..., \quad < \frac{A + iB}{\omega} + \frac{1}{2} \] (49)

and normalized wave functions become

\[ \phi_n(u) = \sqrt{\frac{2\alpha(s - \frac{1}{4})M\omega n!}{\Gamma(n + 2s + \frac{1}{2})}} (M\omega u^2)^{s+\frac{1}{2}} \exp(-M\omega u^2) L_n^{2s+\frac{1}{2}}(M\omega u^2) \] (50)

where \( s = \frac{1}{4} + \frac{1}{2}\sqrt{-2mE}, \quad n = 0, 1, 2, ... \)

V. CONCLUSION

The energy eigenvalues and the corresponding wave functions for PT-/non-PT-Symmetric and non-Hermitian generalized Morse potential are obtained by using Path integral method. The real energy spectra of the PT-/non-PT-symmetric and non-Hermitian forms of potential have been obtained by restricting the potential parameters. The Hamiltonian of system transformed to the form of the two oscillators case with the frequency \( \omega \) with a proper time parameter \( s \). The approach can also be applied to the other PT-/non-PT-Symmetric and non-Hermitian potentials for which the potential problem can be transformed to the oscillator case.

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