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PATH INTEGRAL SOLUTIONS OF PT-/NON-PT SYMMETRIC AND NON-HERMITIAN DENG-FAN MOLECULAR POTENTIAL

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ABSTRACT

In this study, Path integral behavior of Parity-Time (PT)-/non-PT- Symmetric and Non-Hermitian Deng-Fan Molecular potential is examined. Appropriate coordinate and momentum transformations and parametric time were defined and the kernel of the system was found. By applying the path integral method, Green's function, which gives energy eigenvalues and wave functions of the system, is evaluated. Energy eigenvalues and corresponding wave functions of PT- / PT Symmetric and Non-Hermitian systems were obtained.

Keywords: Feynman's Path Integral, Deng-Fan Molecular potential, PT-Symmetry, Non-Hermitian potentials

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1. INTRODUCTION

Path integral formulation of quantum mechanics involves the principle of action in classical mechanics and quantization of the system. This method, obtained by Feynman (Feynman and Hibbs, 2010) is expressed in kernels that give the quantum mechanical amplitude of the point particle at a position x_a at time t_a to reach a position x_b at time t_b. This expression is also related to the energy-dependent Green Function of the Schrödinger equation. Using the Feynman Path integral method, the kernel was derived for various potentials. Duru and Kleinert worked by mapping the three-dimensional Hydrogen atom to the Harmonic oscillator problem with the Kustaanheimo Stiefel transformation (Duru and Kleinert, 1979). The space-time transformation used in this study was used to obtain an exact solution with path integral for various potentials (Duru, 1986; Kandirmaz, 2017; Kandirmaz and Sever, 2009; Kandirmaz and Sever, 2011; Grosche, 2005; Gresche, 1998).

In standard formalism of quantum mechanics, the Hermitian Hamiltonian with real potential has real eigenvalues. In 1998, Bender and Boettcher (Bender and Boetcher, 1998) expressed that the eigenvalues of non-Hermitian Hamiltonian systems with PT symmetry could also be real, which increased the interest in these studies. These studies had the opportunity to apply in many fields of physics such as nuclear physics, condensed matter physics, quantum field theory. Analytical and numerical techniques were used to prove that PT symmetric and non-Hermitian systems have real energy eigenvalues. Path integral method is one of the analytical methods used to obtain an exact solution (Bender and Boetcher, 1998; Bender, 2011; Mostafazadeh, 2002; Arda and Sever, 2014).

In PT-symmetry, $\hat{P}$ is the parity operator acting as space reflection; $\hat{T}$ represents the time reversal operator acting as the complex conjugate operator. In the case where the PT-symmetry is not disturbed, the eigenfunctions of the Hamiltonian are also the eigenfunctions of the PT-operator and the energy spectrum is real. In the case where the PT-symmetry is spontaneously disrupted, the wave functions corresponding to these Hamiltonian, even if the potential is PT-symmetric, are not PT-symmetric and the energy eigenvalues are formed in complex conjugate pairs. However, non-Hermitian, but PT symmetric Hamiltonian systems may have a real spectrum. (Bender and Boetcher 1998, Bender, 2012). Deng-Fan molecular potential was proposed by Deng and Fan in 1957. It is defined by

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$$V(r) = D\left[1 - \frac{b}{e^{\alpha r}-1}\right]^2, b = e^{\alpha r_e} - 1, r \in (0,\infty) \quad (1)$$

and also the shifted Deng-Fan potential is

$$V(r) = D\left[\frac{b^2}{(e^{\alpha r}-1)^2} - \frac{2b}{e^{\alpha r}-1}\right] \quad (2)$$

Where D is the dissociation energy, r_e is the equilibrium inter-nuclear distance and α is the range of the potential well. This potential is the general state of the Morse potential that is structurally related to the Manning-Rosen potential. It is used to describe diatomic molecular energy spectra and electromagnetic transitions. (Rong et al.2003; Diaf, 2015; Hamzavi and Ikhdair, 2013; Dong and Gu, 2018)

The purpose of this paper is to obtain the energy spectrum and the corresponding wave functions of the PT-/Non-PT-Symmetric and Non Hermitian Deng-Fan Molecular Potential using Feynman's Path integral method. This study is organized as follows. In the section 2.1, Feynman path integral formalism which we will use is shown. In 3.1, we have made the kernel of the PT-symmetric system solvable by the Path integral method using coordinate and time transforms. In section 3.2 we have shown the energy eigenvalues and the corresponding wave functions. In section 3.3, we obtained the energy spectrum and wave functions of the PT symmetric and non-Hermitian (1) potential by repeating sections 3.1 and 3.2.

2. MATERIALS AND METHODS

The Lagrange function is defined for a point particle with mass m, moving at a potential V (x) in a dimension

$$L(x,\dot{x};t) = \frac{1}{2}m\dot{x}^2 - V(x,t). \quad (3)$$

(Landau and Lifshitz, 1976). Here, the dynamic variable $x(t)$ shows the classical trajectory of the particle and $\dot{x}(t)$ derivative over time. Hamiltonian, which represents the energy of the system, is also expressed as a total of kinetic and potential energy. Lagrangian is written in the Hamiltonian form as follows

$$L(x,\dot{x};t) = p_x\frac{dx}{dt} - H(x,p_x;t) \quad (4)$$

The action of the system parameterized by t in the $t_1 \leq t \leq t_2$ time interval is defined as

$$S(x,\dot{x};t) = \int_{t_a}^{t_b} dt\, L(x,\dot{x};t). \quad (5)$$

Propagator that carries the system from position x_a to position x_b with the help of time-evolution operatör is

$$\langle x_b, t_b | x_a, t_a\rangle = \left\langle x_b \middle| e^{-i(t_b-t_a)\hat{H}} \middle| x_a \right\rangle. \tag{6}$$

Here $e^{-i(t_b-t_a)\hat{H}}$ is time- evolution operator. The propagator, also called Kernel, is found using the Path integral. It is defined for a point particle with mass m, moving at a potential V (x) in a dimension that reaches from position x_a at time t_a to reach a position x_b at time t_b (Feynman, 2010):

$$K(x_b, t_b; x_a, t_a) = \int \frac{DxDp}{2\pi} exp \frac{i}{\hbar} \int dt[p\dot{x} - \frac{p^2}{2m} - V(x)]. \tag{7}$$

It is also called a propagator because it is a transformation that regulates the time evolution of the system. The kernel containing the Green function is expressed as

$$K(x_b, t_b; x_a, t_a) = \frac{1}{2\pi i\hbar} \int_{-\infty}^{\infty} e^{iET/\hbar}\ G(x_b, x_a; E)dE \tag{8}$$

The discrete form of the kernel divided by the N interval

$$K(x_b, x_a; T) = \lim_{N\to\infty} \int \sum_{j=1}^{N} dx_j \prod_{j=1}^{N+1} \left(\frac{dp_j}{2\pi\hbar}\right) \exp\{\frac{i}{\hbar} \sum_{j=1}^{N+1} [p_j\, \Delta x_j - \frac{p_j^2}{2m} - V(x_j)]\varepsilon\} \tag{9}$$

where $T = t'' - t'.$, $\Delta x_j = x_j - x_{j-1}$, $\varepsilon = t_j - t_{j-1}$, $t' = t_0 = t_a$, $t'' = t_N = t_b$. In this method, which is called Feynman's path integral formalism, we will try to simulate the exact solution of the kernel by using the appropriate coordinate and time transforms for the kernel.

3. RESULTS AND DISCUSSION

3.1. The Kernel of the PT-Symmetric Deng-Fan Molecular Potential

Using $\alpha \to i\alpha$ PT-Symmetric Deng-Fan Molecular Potential is written as

$$V(x) = D\left[\frac{b^2}{(e^{i\alpha x} - 1)^2} - \frac{2b}{e^{i\alpha x} - 1}\right] \tag{10}$$

where D, b are real.

The kernel form in Eq. (5) containing the potential Eq. (6) is

$$K(x_b, x_a; T) = \lim_{N\to\infty} \int \quad \sum_{j=1}^{N} dx_j \sum_{j=1}^{N} \frac{dp_j}{2\pi\hbar} \exp\{\frac{i}{\hbar} \sum_{j=1}^{N+1} [p_j \Delta x_j - \frac{p_j^2}{2m} - D[\frac{b^2}{(e^{i\alpha x} - 1)^2} - \frac{2b}{e^{i\alpha x} - 1}]]\varepsilon\} \tag{11}$$

Coordinate and momentum transformations are

$$e^{i\alpha\alpha x} = -cot^2\theta, \qquad p_x = -\frac{i\alpha}{2} cos\theta sin\theta P_\theta \tag{12}$$

The Jacobian contribution of these transformations is $\alpha sin\theta_b cos\theta_b$. Thus Eq. (7) becomes the form

$$K(\theta_a, \theta_b; T) = -\frac{i\alpha}{2} cos\theta_b sin\theta_b \int D\theta Dp_\theta \exp[i \int dt\, (p_\theta \dot{\theta} + \frac{\alpha^2 cos^2\theta sin^2\theta}{4} \frac{p_\theta^2}{2\mu} - Db^2 sin^4\theta - 2bD sin^2\theta)] \tag{13}$$

Here we have $\hbar = 1$ and μ is the reduced mass. Because of coordinate and momentum transformations, we define a new time parameter to eliminate the multiplier in front of kinetic energy.

$$t = -\frac{4}{\alpha^2} \int \frac{1}{sin^2\theta cos^2\theta} ds \tag{14}$$

The new time parameter can be expressed as the Fourier transform of the Delta function as (Duru and Kleinert, 1979; Duru, 1973; Kandirmaz, 2007; Kandirmaz, 2011)

$$1 = \int dS \int \frac{dE}{2\pi} \frac{4}{\alpha^2 sin^2\theta cos^2\theta} exp\left[i\left(-ET - \int ds \frac{4E}{\alpha^2 sin^2\theta cos^2\theta}\right)\right] \tag{15}$$

where S=s$_b$-s$_a$. Using Eq.(10) and Eq.(11) we can perform Eq.(9) as following

$$K(\theta_a, \theta_b; T) = -\frac{i\alpha}{2} cos\theta_b sin\theta_b \int D\theta Dp_\theta \exp[i \int dt\, (p_\theta \dot{\theta} - \frac{p_\theta^2}{2\mu} + \frac{4Db^2 sin^2\theta}{\alpha^2 cos^2\theta} + \frac{8bD}{\alpha^2 cos^2\theta} - \frac{4E}{\alpha^2 sin^2\theta cos^2\theta})] \tag{16}$$

The endpoint contribution from Jacobien to the kernel is that the kernel in Eq. (5) contains $N+1$ momentum. We can symmetrize this contribution according to points a and b.

$$\frac{1}{sin\theta_b cos\theta_b}=\frac{1}{\sqrt{sin2\theta_a sin2\theta_b}}exp\left(i\int_0^S ds(-i)\frac{cos2\theta}{sin2\theta}\dot{\theta}\right) \tag{17}$$

Thus we can write Eq. (5) as

$$K(x_b,x_a;T)=\int_0^\infty \frac{dE}{2\pi}e^{iET}\int Dse^{\frac{8\mu Db^2}{\alpha^2}S}\frac{1}{i\alpha\sqrt{sin2\theta_a sin2_b}}K(\theta_b,\theta_a;S) \tag{18}$$

here

$$K(\theta_b,\theta_a;S)=\int D\theta Dp_\theta \exp\{i\int_0^S ds\,[p_\theta\dot{\theta}-\frac{p_\theta^2}{2\mu}$$
$$-\frac{1}{2\mu}\left(\frac{\kappa(\kappa-1)}{sin^2\theta}-\frac{\gamma(\gamma-1)}{cos^2\theta}-\frac{ip_\theta cos2\theta}{sin2\theta}\right]\} \tag{19}$$

and κ and γ are

$$\kappa=\frac{1}{2}\left[1+\sqrt{1+\frac{32\mu E}{\alpha^2}}\right],\quad \gamma=\frac{1}{2}\left[1+\sqrt{1-\frac{32\mu}{\alpha^2}(Db^2+2bD-E)}\right]. \tag{20}$$

The following contribution in kernels due to symmetry in Eq.(13) in $\varepsilon\to 0$ limit it is vanished (Duru and Kleinert, 1979; Duru, 1973; Kandirmaz, 2007; Kandirmaz, 2011):

$$\dot{\theta}_j\to\dot{\theta}_j\pm\frac{icos2\theta}{2\mu sin2\theta}\quad or\qquad \frac{\theta-\theta_{j-1}}{\in}\to\frac{\theta_j-\theta_{j-1}}{\in}\pm\frac{ip_\theta cos2\theta}{2\mu sin2\theta}. \tag{21}$$

Eq. (15) is the kernel of the Pöschl Teller potential. Using the solutions of the Pöschl Teller potential, we can directly write the solution of the PT-Symmetric Molecular Deng-Fan Oscillator potential. The kernel is expressed in terms of the wave function as

$$K(\theta_b,\theta_a;S)=\sum_{n=0}^{\infty}e^{-i(\frac{S}{2\mu})(\kappa+\gamma+2n)^2}\psi_n(\theta_a)\psi_n^*(\theta_b). \tag{22}$$

3.2. Energy Spectrum and Wave functions for PT-Symmetric Deng-Fan Molecular Potential

The energy spectrum of PT symmetric Deng-Fan molecular potential is obtained as

$$E_n = Db^2 + 2bD - \frac{\alpha^2}{32\mu} + \left[\frac{\alpha^2}{32\mu}\frac{[\frac{8\mu}{\alpha^2}(Db^2+2bD) - (2n+1-\sqrt{\frac{8\mu Db^2}{\alpha^2}})^2]}{(2n+1-\sqrt{1+\frac{8\mu Db^2}{\alpha^2}})^2}\right]^2 \tag{23}$$

and normalized wave functions in terms of Jacobi polynomials (Grosche, 2005; Grosche, 1989; Kleinert and Mustapic, 1992) are

$$\psi_n(\theta) = \sqrt{2(\kappa+\gamma+2n)}\sqrt{\frac{\Gamma(n+1)\Gamma(\kappa+\gamma+n)}{\Gamma\left(\kappa+n+\frac{1}{2}\right)\Gamma\left(\gamma+n+\frac{1}{2}\right)}}(cos\theta)^{\gamma}(sin\theta)^{\kappa}$$

$$\times P_n^{\left(\kappa-\frac{1}{2},\ \gamma-\frac{1}{2}\right)}(1-2sin^2\theta) \tag{24}$$

κ and γ are found in Eq. (16). If we add the Eq. (15) in the Eq. (11) and then integrate over S, then the kernel is as

$$K(x,x_a;T) = \frac{-1}{i\alpha\sqrt{sin2\theta_a sin2\theta_b}}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\frac{dE}{2\pi\pi}\frac{e^{iET}}{(\kappa+\gamma-2n)^2-1}\psi_n(\theta_a)\psi_n^*(\theta_b). \tag{25}$$

Thus, we obtain the energy eigenvalues and wave functions of the system as follows

$$\varphi(x) = \frac{i}{2\sqrt{2}\sqrt{n+1}}\sqrt{4(n+1)^2-(\gamma_n-\kappa_n)^2}\sqrt{\frac{\Gamma(n+1)\Gamma(-n-1)}{\Gamma\left(\kappa_n+n+\frac{1}{2}\right)\Gamma\left(\gamma_n+n+\frac{1}{2}\right)}}$$

$$\times\frac{\exp[(\kappa_n-\frac{1}{2})\,i\alpha x]}{(e^{i\alpha x}+1)^{\left(\kappa_n+\gamma_n-\frac{1}{2}\right)}}P_n^{(\kappa_n-\frac{1}{2},\gamma_n-\frac{1}{2})}\left(\frac{e^{i\alpha x}+1}{e^{i\alpha x}-1}\right) \tag{26}$$

where

$$\kappa_n = \frac{1}{2} + Db^2 + 2bD - \frac{\alpha^2}{32\mu}[(2n+1-\sqrt{1+\frac{8\mu Db^2}{\alpha^2}}) + \frac{\frac{8\mu}{\alpha^2}(Db^2+2bD)}{2n+1-\sqrt{1+\frac{8\mu Db^2}{\alpha^2}}}] \tag{27}$$

and

$$\gamma_n = \frac{1}{2} + Db^2 + 2bD - \frac{\alpha^2}{32\mu}[\left(2n+1-\sqrt{1+\frac{8\mu Db^2}{\alpha^2}}\right) - \frac{\frac{8\mu}{\alpha^2}(Db^2+2bD)}{2n+1-\sqrt{1+\frac{8\mu Db^2}{\alpha^2}}}]. \tag{28}$$

We see that PT Symmetric Deng-Fan Molecular potential has real energy eigenvalues. We can see that these results coincide with the results in ref. (Diaf, 2015; Hamzavi et al. 2013; Dong and Gu, 2008)

3.3. Non-PT-Symmetric and Non-Hermitian Deng-Fan Molecular potential

Non-PT-Symmetric and Non-Hermitian Deng-Fan Molecular potential is determined by taking $D \to A + iB$ and $\alpha \to i\,\alpha$. Following the same steps in Sections (3.1) and (3.2), we obtain the energy eigenvalues and corresponding wave functions for the Non-PT-Symmetric and Non-Hermitian Deng-Fan Molecular potential. Discrete form of kernel for this potential is

$$K(x_b, x_a; T) = \lim_{N\to\infty} \int \sum_{j=1}^{N} dx_j \sum_{j=1}^{N} \frac{dp_j}{2\pi\hbar} \exp\{\frac{i}{\hbar} \sum_{j=1}^{N+1} [p_j \Delta x_j - \frac{p_j^2}{2m} - (A + iB)[\frac{b^2}{(e^{i\alpha x}-1)^2} - \frac{2b}{e^{i\alpha x}-1}]]\varepsilon\}. \tag{29}$$

By taking the appropriate coordinate and momentum transformation, we can write the kernel as follows

$$K(\theta_a, \theta_b; T) = -\frac{i\alpha}{2} cos\theta_b sin\theta_b \int D\theta Dp_\theta \, exp[i \int dt \, (p_\theta \dot{\theta} - \frac{p_\theta^2}{2\mu} - \frac{4(A+iB)b^2 sin^2\theta}{\alpha^2 cos^2\theta} - \frac{8b(A+iB)}{\alpha^2 cos^2\theta} - \frac{4E}{\alpha^2 sin^2\theta cos^2\theta})]. \tag{30}$$

Parametric time is defined as

$$t = \frac{1}{\alpha^2} \int \frac{ds}{sin^2\theta cos^2\theta}. \tag{31}$$

If we follow the steps in Sec. (3.2) we obtain energy eigenvalues of Non-PT-Symmetric and Non-Hermitian Deng-Fan molecular potential as

$$E_n = (A+iB)b^2 + 2b(A+iB) - \frac{\alpha^2}{32\mu}$$

$$+\left[\frac{\alpha^2}{32\mu}\frac{[\frac{8\mu}{\alpha^2}((A+iB)b^2+2b(A+iB)) - (2n+1-\sqrt{\frac{8\mu(A+iB)b^2}{\alpha^2}})^2]}{(2n+1-\sqrt{1+\frac{8\mu(A+iB)b^2}{\alpha^2}})^2}\right]^2 \qquad (32)$$

κ_n and γ_n same in Eq. (22). It is seen that energy spectrum has complex eigenvalues.

4. CONCLUSION

In this study, we obtained the energy spectrum and normalized wave functions of PT/non-PT Symmetric and Non-Hermitian Deng Fan Molecule function by using Path integral method developed by Duru and Kleinert. By defining space-time transformations, we derived the parametric time kernel of the system. We have obtained the Green function of the system by converting the kernel solutions we derived to the kernels of the well-known Pöschl-Teller potential. We found the energy and wave functions of Green's function and the energy eigenvalues and the corresponding wave functions for the PT /non-PT symmetric Deng Fan molecular potential.

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