Arbitrary $\ell$-state solutions of the Feynman propagator with the Deng-Fan molecular potential

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Abstract. The bound state solutions of the Feynman propagator with the rotating Deng-Fan molecular potential are presented approximately. An approximation of the centrifugal potential is used and nonlinear space-time transformations are applied. A relation between the original path integral and the Green function of a new quantum soluble system is derived. The energy spectrum and the normalized eigenfunctions are both obtained for the application of this technique to the Deng-Fan molecular potential. Our results are in very good agreement with those found by using numerical and other methods.

1. Introduction
The exact analytical solution of the Schrödinger equations are only possible with the angular momentum $\ell = 0$ for some potential models. However, when $\ell \neq 0$ [1, 2], the Schrödinger equation can only be solve approximately for different suitable approximation scheme [3, 4]. This is due to the presence of the centrifugal term $(1/r^2)$. Motivated by the success in obtaining approximately the bound state solutions of the Feynman propagator with the Manning-Rosen and the Rosen-Morse potentials [5, 6], we attempt here to solve the arbitrary $\ell$-wave propagator with the Deng-Fan potential [7]. An improved approximation scheme for the centrifugal term is used as in [4] and non linear space-time transformations are applied.

The Deng-Fan ($D-F$) potential is given by

$$V_{D-F}(r) = D \left(1 - \frac{be^{-\alpha r}}{1-e^{-\alpha r}}\right)^2. \tag{1}$$

where $0 \leq r < \infty$, $b = e^{\alpha r_c} - 1$, the three parameters $D$, $b$, and $\alpha$ denote the dissociation energy, the position of the minimum $r_c$, and the range of the potential, respectively. This potential has been one of the most useful and convenient models to study the energy eigenvalues and electromagnetic transitions of diatomic molecules. It is known that for this potential, the Schrödinger equation can be solved exactly when $\ell = 0$ either directly [8] or by using SO(2, 1) algebra method [9]. Unfortunately, for arbitrary $\ell$-state, the radial Schrödinger equation does not admit exact solutions. In this case, some authors have used the approximation scheme proposed by Lu [3] to study analytically arbitrary $\ell$-state bound states of the Schrödinger equation for the Deng-Fan potential [11].

This paper is organized as follows. In Sec. 2 we derive arbitrary $\ell$-states solutions of the Deng-Fan potential within the Feynman path integrals formalism by approximate method. In Sec.3...
the numerical calculations are given to compare with those obtained by other method. The concluding remarks are given in Sec. 4.

2. Green’s function

The propagator for a particle of mass \( m \) in the spherically symmetric potential, can be developed into a sum of partial waves of the form [10]:

\[
K(\vec{r}''', \vec{r}''; \vec{r}', t') = \frac{1}{4\pi r''r'} \sum_{l=0}^{\infty} (2l + 1) K_l(r''', r''; r', t') P_l(\cos \theta). \tag{2}
\]

\( P_l(\cos \theta) \) is the Legendre polynomial with \( \theta \equiv (\vec{r}'', \vec{r}'') \) and

\[
K_l(r''', r''; r', t') = \lim_{N \to \infty} \int \prod_{j=1}^{N} \exp \left[ \frac{i}{\hbar} S_j \right] \prod_{j=1}^{N} \left[ \frac{m}{2\pi \hbar} \right] \frac{1}{2} \prod_{j=1}^{N-1} dr_j. \tag{3}
\]

Here \( S_j = \frac{m}{2\pi} (\Delta r_j)^2 - \varepsilon V_{\text{eff}}(r_j), \) where

\[
V_{\text{eff}}(r_j) = \frac{\hbar^2}{2m} \frac{l(l+1)}{r_j r_{j-1}} - \frac{V_1}{\cosh^2(r_j/a)} + V_2 \tanh(r_j/a) \tag{4}
\]

and \( \Delta r_j = r_j - r_{j-1}, \varepsilon = t_j - t_{j-1}, t' = t_0 \) and \( t'' = t_N. \) Moreover, setting \( T = t'' - t' \), we can write:

\[
K_l(r'', r', T) := K_l(r'', r''; r', t'). \tag{5}
\]

To calculate the propagator \( K_l \) given by equation (3) for \( l \neq 0 \) states, we apply the following approximate scheme to the centrifugal term [4] :

\[
\frac{1}{r^2} \approx 4\alpha^2 \left[ C_0 + \frac{e^{-2\alpha r}}{1 - e^{-2\alpha r}} + \left( \frac{e^{-2\alpha r}}{1 - e^{-2\alpha r}} \right)^2 \right], \tag{6}
\]

where the parameter \( C_0 = 0.08230581867837972 \) is a shift determined by the expansion procedures. By substituting the centrifugal term in (4) by its approximation (6), we get

\[
V_{\text{eff}}(r_j) = A \tanh(2\alpha r_j) - \frac{B}{\cosh^2(2\alpha r_j)} + C, \tag{7}
\]

with \( A = bD + \frac{D_b^2}{2}, B = \frac{l(l+1)\alpha^2}{4m} + \frac{D_b^2}{4} \) and \( C = \frac{C_0 l(l+1)\alpha^2}{4m} + (b + 1)D + \frac{D_b^2}{2}. \)

In the following, we study the potential (7) with the Duru-Kleinert method [12]. The path integral for the potential (7) is

\[
K_l(r'', r'; T) = \int \mathcal{D}r(t) \exp \left[ \int_{t'}^{t''} \left( \frac{m}{2} \dot{r}^2 - V_{\text{eff}}(r) \right) dt \right]. \tag{8}
\]

By achieving the point canonical transformation and the time transformation [8],

\[
\begin{cases}
  r &= \tilde{f}(q) \\
  dt &= [f'(q)]^2 d\xi,
\end{cases} \tag{9}
\]

In our case, we choose

\[
r = \left( \frac{1}{\alpha} \right) \text{arccoth}(2 \coth^2 q - 1), \tag{10}
\]
The propagator expression becomes [11]:
\[
\hat{K}_i(q'', q'; s'') = \exp \left[ \frac{i}{\hbar} s'' \frac{E - C + A}{\alpha^2} \right] 
\times \int Dq(s) \exp \left[ \frac{i}{\hbar} \int_0^{s''} \left( \frac{m}{2} q^2 - \frac{\hbar^2}{2m} \left[ \frac{\eta(n - 1)}{\sinh^2 q} - \frac{\nu(v - 1)}{\cosh^2 q} \right] \right) ds \right]
\]
\[
= \exp \left[ \frac{i}{\hbar} s'' \frac{E - C + A}{\alpha^2} \right] K_{i}^{\text{MPT}}(q'', q'; s'')
\]
(11)
with \( \eta = \frac{1}{2} \pm \sqrt{1 + \frac{8mB}{\alpha^2 \hbar^2}} \), \( \nu = \frac{1}{2} \pm \sqrt{\frac{2m(E - C - A)}{\alpha^2 \hbar^2}} \) and \( K_{i}^{\text{MPT}} \) is the path integral of the modified Pöschl-Teller potential which is a known solved problem [13] for which the bound states wave functions are explicitly given by:
\[
\chi_{l,n}^{(k_1,k_2)}(q) = N_n^{(k_1,k_2)}(\sinh q)^{2k_2-1/2}(\cosh q)^{-2k_1+3/2} \times \mathcal{F}_1(-k_1+k_2+k, -k_1+k_2-k+1; 2k_2; -\sinh^2 q),
\]
where \( k = k_1 - k_2 - n \), and
\[
N_n^{(k_1,k_2)} = \frac{1}{\Gamma(2k_2)} \left( \frac{(2k_1-k_2-k)\Gamma(k_1+k_2+k-1)}{\Gamma(k_1-k_2+k)\Gamma(k_1-k_2-k+1)} \right)^{1/2},
\]
(13)
The eigenvalues are expressed by
\[
E_{n}^{\text{MPT}} = -\frac{\hbar^2}{2m} \left[ 2(k_1 - k_2 - n) - 1 \right]^2.
\]
(14)
Calculating \( \hat{K}_i(q'', q'; s'') \) allows us to obtain the Green function. Since this is known, the whole energy spectrum is obtained from its poles, and from the residues at the poles we obtain the corresponding wave functions.

Substituting (12) in (11), we get
\[
\hat{K}_i(q'', q'; s'') = \sum_{n=0}^{N_m} \exp \left\{ \frac{i}{\hbar} s'' \left[ (E - C + A)(2a)^2 - E_{n}^{\text{MPT}} \right] \right\} \chi_{l,n}^{(k_1,k_2)}(q'') \chi_{l,n}^{(k_1,k_2)}(q')
\]
\[
+ \int_0^\infty dK \exp \left\{ \frac{i}{\hbar} s'' \left[ (E - C + A)(2a)^2 - \frac{\hbar^2 K^2}{2m} \right] \right\} \chi_{l,n}^{(k_1,k_2)}(q'') \chi_{l,n}^{(k_1,k_2)}(q')
\]
(15)
Then, by integrating this latter over the pseudo-time parameters \( s'' \), the Green function \( G \) is written as:
\[
G_i(r'', r'; E) = \sum_{n=0}^{N_n} \frac{D F_{i(n)}^{(k_1,k_2)}(r'')}{E_{n}^{\text{MPT}} - E} \chi_{l,n}^{(k_1,k_2)}(r'') \chi_{l,n}^{(k_1,k_2)}(r')
\]
\[
+ \int_0^\infty dK \frac{\chi_{l,n}^{(k_1,k_2)}(r'') \chi_{l,n}^{(k_1,k_2)}(r')}{(\hbar^2 K^2/2m(2a)^2) - A + C - E}
\]
(16)
Following [13], the values of \( k_1, k_2 \), satisfying the appropriate boundary conditions for \( r \to 0 \) and \( r \to \infty \), are respectively:
\[
k_1 = \frac{1}{2} \left[ 1 + \frac{1}{2} \left( s + 2n + 1 \right) + \frac{2mA}{\alpha^2 \hbar^2 (s + 2n + 1)} \right]
\]
\[
k_2 = \frac{1}{2} \left( 1 + \sqrt{1 + \frac{8mB}{\alpha^2 \hbar^2}} \right) \equiv \frac{1}{2} (1 + s)
\]
(17)
Substituting these values of \( k_1, k_2 \) in (12) and (14), and by considering \( u = \frac{1}{2} [1 - \tanh(2\alpha r)] \), we get

\[
\chi_{n,\ell}^{DF}(k_1,k_2)(r) = \sqrt{\alpha} \frac{N_n(k_1,k_2)(1 - u)^{\frac{1}{2}}}{2^{k_1+n}} \left[ \frac{\Gamma(n+s+1)\Gamma(2k_1-s-n-1)}{\Gamma(n+1)\Gamma(2k_1-n-1)} \right]^{1/2} \left(1 - e^{-2r}\right)^{k_2} \times \exp\left\{-2r \left[k_1 - \frac{s}{2} - n - 1\right]\right\} P_n^{(2k_1-2n-s-2,s)}(1 - 2e^{-2r})
\]

The energy spectrum is obtained from the poles,

\[
E_{n,\ell}^{DF} = \alpha^2 E_{n}^{MPT} - A + C
\]

\[
= - \left[ \frac{\hbar^2}{8m} \alpha^2 (s + 2n + 1)^2 + \frac{2mA^2}{\hbar^2 \alpha^2 (s + 2n + 1)^2} \right] + C
\]

3. Results and discussions

Energies calculated by using the path integral method described above are reported in the Table. the results, Eq. (20) are displayed in Table hereafter, where a comparison is made with the calculations of Dong et al [14], who solved analytically the Schrödinger equation, but using another approach for the centrifugal barrier. All results are compared to the numerical data [1]. Our results are almost indistinguishable from the numerical ones [1]. Nevertheless, except in a few cases, we get results closer to the numerical estimates compared to the method of Dong [14]. This is due to our choice of the centrifugal barrier.

4. Concluding remarks

In this paper, we have presented a path integral treatment for the Deng-Fan potential. By Using an approximation scheme for the centrifugal term and a nonlinear space-time transformations in the radial path integral, We were able to derive explicit expressions of the wave functions in terms of Jacobi polynomials and the energy eigenvalues in function of the potential parameters. The barrier approximation being fixed, we note that the Feynman integral method gives results closer to numerical one than solving the Schrödinger equation.

To conclude, our method is efficient in solving this type of potentials. We intend in a near future, to expand the path integral method to a more general form of potentials and relativistic cases.

References

[1] L. D. Landau and E. M. Lifshitz (1977) Quantum Mechanics, Non-Relativistic Theory, Pergamon, Oxford.
[2] L. I. Schiff (1955) Quantum Mechanics 3rd edition, McGraw-Hill, New York.
[3] R. L. Greene and C. Aldrich, Phys. Rev. A 14 (1976)2363.
[4] S. M. Ikhdair and R. Sever, Ann. Phys. (Berlin) 18, No. 4 (2009)189 197.
[5] A. Diaf, A. Chouchaoui and R.L. Lombard, Ann. Phys. 317, (2005) 354.
[6] A. Diaf and A Chouchaoui, Phys. Scr. 84, (2011) 015004.
[7] Deng, Z. H., Fan, Y. P. Shandong Univ J 7(1957) 162.
[8] Mesa, A. D. S.; Quesne, C.; Smirnov, Y. F. J Phys A: Math Gen, 31(1998), 321.
[9] Codriansky, S.; Cordero, P.; Salamo , S. J Phys A: Math Gen, 32(1999)6287.
[10] D. C. Khandekar, S.V. Lawande, K.V. Bhagwat, Path Integral Methods and their Applications ( World Scientific, Singapore,1986)
[11] Dong, S. H.; Gu, X. Y. J Phys: Conf Ser 2008, 96, 012109.
Table 1. Eigenvalues $-E_{n,l}$ of the Deng-Fan potential in atomic units ($\hbar = m = 1$) with $D = 15$ and $r_e = 0.4$.

| States | $\alpha$ | Present | Dong et al[14] | Lucha et al[15] |
|--------|---------|---------|---------------|----------------|
| 2p     | 0.05    | 7.86080 | 7.86060       | 7.8628         |
|        | 0.1     | 7.95329 | 7.95247       | 7.95537        |
|        | 0.15    | 8.04508 | 8.04322       | 8.04724        |
|        | 0.2     | 8.13613 | 8.13287       | 8.13842        |
|        | 0.25    | 8.22655 | 8.22142       | 8.22892        |
|        | 0.3     | 8.31629 | 8.30889       | 8.31874        |
| 3p     | 0.05    | 10.99776| 10.9976       | 10.9998        |
|        | 0.1     | 11.16255| 11.1617       | 11.1647        |
|        | 0.15    | 11.32422| 11.3224       | 11.32647       |
|        | 0.2     | 11.48280| 11.4795       | 11.48513       |
|        | 0.25    | 11.63827| 11.6331       | 11.64068       |
|        | 0.3     | 11.79066| 11.7833       | 9.67565        |
| 3d     | 0.05    | 10.21597| 10.2154       | 10.21654       |
|        | 0.1     | 10.35350| 10.3510       | 10.35409       |
|        | 0.15    | 10.48928| 10.4837       | 10.48992       |
|        | 0.2     | 10.62334| 10.6135       | 10.62403       |
|        | 0.25    | 10.75571| 10.7403       | 10.75645       |
|        | 0.3     | 10.88644| 10.8642       | 10.88719       |
| 4p     | 0.05    | 12.49760| 12.4974       | 12.4992        |
|        | 0.1     | 12.69678| 12.6960       | 12.69851       |
|        | 0.15    | 12.88832| 12.8865       | 12.8901        |
|        | 0.2     | 13.07220| 13.0689       | 13.07400       |
|        | 0.25    | 13.24840| 13.2433       | 13.2501        |
| 4d     | 0.05    | 12.09828| 12.0977       | 12.0989        |
|        | 0.1     | 12.28498| 12.2825       | 12.2857        |
|        | 0.15    | 12.46635| 12.4608       | 12.46715       |
|        | 0.2     | 12.64244| 12.6326       | 12.64324       |
| 4f     | 0.05    | 11.82077| 11.8195       | 11.8209        |
|        | 0.1     | 11.99790| 11.9930       | 11.9981        |
|        | 0.15    | 12.17156| 12.1604       | 12.1718        |
|        | 0.2     | 12.34182| 12.3221       | 12.3421        |
|        | 0.2     | 13.54213| 13.5413       | 13.5434        |
| 5p     | 0.1     | 13.92894| 13.9257       | 13.9301        |

[12] H. Kleinert, Path integrals in Quantum Mechanics, Statistics and Polymer Physics, World scientific, Singapore, 2009.
[13] C. Groshe J. Phys. A. Math. Gen. 22, (1989) 5073.
[14] Dong, S. H.; Gu, X. Y. J Phys: Conf Ser , 96(2008)012109.
[15] W. Lucha and F.F. t. J. Mod. Phys. C 10, (1999)607.