Time-correlation function and average energy of molecules in presence of Deng-Fan potential in a moving boundary

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Abstract For the Deng-Fan potential within a moving boundary condition, the time-dependent Schrödinger equation is considered analytically. The eigenvalue equation is solved by using a combination of Pekeris and Greene-Aldrich approximations. Various time-dependent quantities including density distribution function, auto-correlation function, disequilibrium, average energy, quantum similarity, and quantum similarity index are obtained for selected eight diatomic molecules. The motion of the peak of the density function, with moving boundary condition is investigated for ground states of some diatomic molecules along with the corresponding peak values.

Keywords Deng-Fan potential · Ro-vibrational energy · Average energy · Time-correlation function · Auto-correlation function · Quantum similarity index · Moving boundary

1 Introduction

For a proper understanding of molecule, an accurate and reliable potential energy function (against interatomic distance) is essential. Ever since the publication of first three-parameter, analytical potential [1], perhaps the oldest one, a plethora of attempts have been made to design progressively better functions. The correct knowledge about their eigenvalues and eigenfunctions leads to valuable information regarding transition frequency and matrix elements. An ideal potential function should satisfy the following limiting conditions at small and large distances, namely, $V(0) = \infty$ and remains a constant as $r \to \infty$. While Morse potential suffers from certain limitations (e.g., remains finite at $r \to 0$) and thus exhibits considerable disagreements with experimental observations, it does provide a basis for construction of improved functions. This has remained an active area of research covering a large span of time, with widespread applications in molecular spectroscopy atom/molecule adsorption on solid surface, deformation of cubic metal, etc. Some important and popular models for vibrational interactions in molecules are as follows: Manning-Rosen [2–5], Hülthen [6–9], Woods-Saxon [10,11], Pöschl-Teller [5,12,13], Tietz-Hua [14–16], pseudoharmonic [17–19], Rosen-Morse [20–22], Kratzer [23,24], Eckart [25] and so on.

In the current work, we focus on yet another potential function, namely, Deng-Fan (DF) potential for diatomic molecules, which was introduced about 70 years ago. Being a three-parameter function, it can be expressed as below
where the (+)ve parameters $D_e, r_e, \alpha$ refer to dissociation energy, equilibrium internuclear distance and potential well radius. In the limit of internuclear distance approaching zero and infinity, it provides a qualitatively correct behaviour. Due to its close resemblance to Morse potential, it is often referred as Generalized Morse potential [26,27]. Its connection to another important diatomic potential (Manning-Rosen) has been discussed as well. A shifted (by dissociation energy) sDF potential [28] has generated much interest in the literature in recent years. For large $r$ region ($r \approx r_e, r > r_e$), it closely resembles the Morse potential, but differs at $r \approx 0$. Also, the deep ($D_e \gg 1$), DF and sDF potentials can be approximated by harmonic oscillator in $r \approx r_e$ region [26].

For an arbitrary angular momentum state, the eigenvalues and eigenfunctions cannot written down in closed analytical form exactly. Thus various approximations were reported in relativistic and non-relativistic domain; the literature is quite vast. We mention here some prominent ones. The exact solvability problem has been addressed in [26] via an $SO(2, 2)$ symmetry algebra. The circular, nodeless states were studied by algebraic method [29]. Approximate analytical eigensolutions for rotating DF potential were expressed in terms of generalized hyper-geometric functions $2F_1(a, b; c; z)$ [30] in a given quantum state. Within a super-symmetric shape invariance method, an improved approximation to the centrifugal term was adopted in [31]. An analytical solution for Dirac equation has been reported within the above method [32]. In [33], solutions of Klein-Gordon equation for nonzero-$\ell$ states were discussed. In another attempt, a Pekeris approximation for centrifugal term within a Nikiforov-Úvarov (NU) framework was advocated for Dirac, Klein-Gordon as well as Schrödinger equation (SE) [28,34,35]. The Klein–Gordon equation in $D$-dimension was treated by means of an ansatz method in bound states [36], while scattering states were reported in [37]. Accurate results were reported by means of numerical generalized pseudospectral [38] method. Apart from these, one can also find exact quantization rule [39], as well as a Feynman path-integral formalism [40] coupled with an approximation for centrifugal term, for the generalized $D$-dimensional problem.

Expectation values [39] and thermodynamic properties [41,42] were also considered. For a critical and comparative analysis of the performance of Morse, Manning-Rosen, Schlöberg and DF potential in the context of diatomic molecules, one may consult [43].

In this communication, at first, we find exact solution of time-dependent (TD) SE in presence of DF potential with moving boundary condition. For quantum systems, time-dependent Schrödinger equation is of great general interest in the linear as well as non-linear domain [44-46]. In this article, we have considered the latter with moving boundary condition. Then we obtain analytical expressions of certain expectation values and time-dependent average energy. Then we pursue a host of time-dependent quantities including time-correlation function, quantum similarity between two states and disequilibrium of a given state. For illustration, we report numerical values of these quantities in case of eight representative diatomic molecules, viz., H$_2$, LiH, HCl, ScH, TiH, CrH, VH and CO. Moreover, we also compute the quantum similarity index (QSI) between two diatomic molecules. In Sect. 2, we describe the theoretical methodology of the time-dependent problem in quantum system with moving boundary condition. In Sect. 3, we make a detailed presentation of the results along with a discussion in the context of these molecules. Finally, we conclude with a few remarks in Sect. 4.

### 2 Theoretical methodology

In this article, we are interested in the time-dependent Schrödinger equation (TDSE), as below

$$\left[ -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} + V(x, t) \right] \psi(x, t) = i\hbar \frac{\partial \psi(x, t)}{\partial t},$$

(2)

where the symbols have their usual meanings. The particular TD potential used here has following form [47,48]:

$$V(x, t) = \frac{1}{L(T)} \bar{W}_{eff} \left( \frac{x-x_0\beta(T)}{L(T)} \right) + \frac{\mu \alpha}{2\mu_0^2} F_1(T)x^2 + \frac{\mu \alpha \gamma}{\mu_0^2} F_2(T)x$$

$$+ \frac{\mu \alpha}{\mu_0} F_3(T), \quad x > x_0\beta(T)$$

$$= \infty, \quad x \leq x_0\beta(T)$$

(3)

where $x_0$ and $t_0$ are scale factors of $x$ and $t$ such that $X = x/x_0, T = t/t_0$; $c$ signifies speed of light and $\hbar$ is the reduced Planck constant. The quantities
The functions $\beta$ and $L$ are dimensionless scale functions of $T$, while the function $x_0 \beta(T)$ represents the moving boundary condition of solutions of TDSE (2). Equation (2) is solvable in presence of the TD potential, Eq. (3) by the method of invariant, provided $L(T)$, $\beta(T)$, $F_1(T)$ and $F_2(T)$ satisfy the Ermakov equation [47–49]. Then the corresponding TD quantum system will be adiabatic.

Here, we have chosen the effective potential $\tilde{V}_{eff}$ to be of DF type, defined in Eq. (1) and a transformation $r = (x - x_0 \beta(T))/L(T)$. Then the corresponding time-independent (TI)SE can be recast in the following form:

$$\frac{h^2}{2\mu} \frac{d^2 Q}{dr^2} + \tilde{V}_{eff}(r) Q(r) = e^{(i)} Q(r)$$

and the TDSE, Eq. (2) becomes solvable, when the following relations hold [49,50]

$$F_1(T) = -\frac{\tilde{L}(T)}{L(T)},$$
$$F_2(T) = \frac{\beta(T)}{L(T)} - \tilde{\beta}(T),$$
$$F_3(T) = \beta(T)\tilde{\beta}(T) - \frac{\beta(T)L(T)}{2L(T)}.$$

where $e^{(i)}$ is the separation constant, which is equal to the eigen spectrum of the TISE. The variables $x$ and $r$ are defined as the TD and time-independent position variables, respectively. Naturally, the corresponding TD potential and the time-independent effective potentials are connected via Eq. (3). It has been shown that the exact solution of Schrödinger equation, under such a condition, can be defined by point transformation and separation of variables [49–68]. Note that the “effective” potential includes the centrifugal term,

$$\tilde{V}_{eff}(r) = V_{DF}(r) + \frac{\ell(\ell + 1)h^2}{2\mu r^2},$$

$$= D_e \left(1 - \frac{\xi}{e^{\alpha r} - 1}\right)^2 + \frac{\ell(\ell + 1)h^2}{2\mu r^2},$$

$$\xi = e^{\alpha r} - 1, \ r \geq 0.$$  

Then the corresponding TD potential is given as

$$V(x, t) = \frac{1}{L(T)^2} \left[V_{DF}(r) + \frac{\ell(\ell + 1)h^2}{2\mu r^2}\right] + \frac{\mu}{2\hbar^2} L^2 F_1(T)r^2 - \frac{\hbar^2}{2\hbar^2} (L(T)\tilde{\beta}(T)) r, \ x > x_0 \beta(T),$$

$$= 0, \ x \leq x_0 \beta(T).$$

It may be noted that DF potential is one of the many molecular potentials reported in the literature, over the past several decades. And its merits and demerits in the context of molecular spectroscopy have been well documented in the references [28–42]. The three parameters present in the potential represent a given molecular system. The particular moving boundary condition can be applicable to other potentials as well; for example, recently it has been applied to Pöschl–Teller potential [50]. It is well known that the DF potential satisfies [69] the conditions given in [70], namely

$$\lim_{r \rightarrow \infty} V_{DF}(r) - V_{DF}(r) = D_e, \left[\frac{dV_{DF}(r)}{dr}\right]_{r=r_e} = 0,$$

$$\left[\frac{d^2 V_{DF}(r)}{dr^2}\right]_{r=r_e} = K_e = 4\pi^2 \mu e^2 \omega_e^2,$$

where $\omega_e$ denotes harmonic vibrational frequency. From Eq. (9), one can find the value of $\alpha$ as below,

$$\alpha = \pi \omega_e \sqrt{\frac{2\mu}{D_e}}$$

$$+ \frac{1}{r_e} \mathcal{P}_L \left[-\pi \omega_e r_e \sqrt{\frac{2\mu}{D_e}} - \frac{\pi \omega_e r_e \sqrt{\frac{2\mu}{D_e}}}{\mathcal{P}_L[ze^{\alpha r}]}ight]$$

where $\mathcal{P}_L[z]$ is the Product log function [71], and it is the principal solution for $w$ in $z = we^w$. Then the TISE is

$$-\frac{h^2}{2\mu} \frac{d^2 Q}{dr^2} + \left[\frac{d}{dr} \left(1 - \frac{\xi}{e^{\alpha r} - 1}\right)^2 + \frac{\ell(\ell + 1)h^2}{2\mu r^2}\right] Q = e^{(i)} Q,$$

and the TI boundary conditions are: $Q(r = 0) = 0$, $\lim_{r \rightarrow \infty} Q(r) = 0$, while the corresponding TD moving boundary conditions are: $\psi(x_0 \beta(T), t) = \lim_{x \rightarrow \infty} \psi(x, t) = 0$. The above equation can be easily solved in the range $(0, \infty)$. However, when a TD moving boundary condition is applied, Eq. (4) is no longer solvable in the standard manner, because this changes the initial condition on the wave function. If we apply the transformations $\psi(x, t) = \mathcal{Z}(r) e^{i\phi(r, T)}$, $r = (x - x_0 \beta(T))/L(T)$, and a separation of variables of the form $\mathcal{Z}(r, T) = \frac{Q(r)\ell(L(T))}{\sqrt{L(T)}}$, where

$$\phi(r, T) = a(T)r^2 + b(T)r + c_1(T),$$

$$a(T) = \frac{\mu}{2\hbar^2} L(T)\tilde{L}(T), b(T) = \frac{\mu x_0}{\hbar^2} L(T)\tilde{\beta}(T),$$

$$c_1(T) = \frac{\mu x_0}{2\hbar^0} \int_0^T \tilde{\beta}^2(s) \, ds,$$

$$\tau(T) = \exp \left\{-\frac{ie^{(i)} t_0}{\hbar} \int_0^T \frac{1}{L^2(s)} \, ds\right\}.$$
then TD Schrödinger equation can be solved (in order to get the TD average energy, average force and position expectation, etc.) in presence of the potential defined in Eq. (3), or equivalently in Eq. (7).

The solutions of Eq. (10) are obtained within a recently proposed scheme combining both Pekeris [72] and Greene-Aldrich [73] approximations. This has lead to a very satisfactory treatment of potential throughout the whole domain of consideration [5,25,42,74,75]. Therefore, solution of Eq. (10) can be expressed as [42],

\[
Q_{n,\ell}(r) = \sqrt{\alpha} N_{n,\ell} \xi_{n,\ell}(1-s) L_1^{(1)} F_1(-n, n + 2\xi_{n,\ell} + 2L_1; 2\xi_{n,\ell} + 1; s), \quad s = e^{-ar},
\]

and energy given by,

\[
\epsilon_{n,\ell}^{(i)} = d_4 = -\frac{a^2 h^2}{2\mu} \frac{d_2^2}{(n+L_1)^2} + \frac{(n+L_1)^2}{4},
\]

where

\[
N_{n,\ell} = \left[ \sum_{k_1, k_2=0}^{n} \frac{(-\bar{n})_{k_1} k_1! (n + 2\xi_{n,\ell} + 2L_1)_{k_1} \Gamma(2\xi_{n,\ell} + k_1 + 2k_2)! \Gamma(2L_1 + 1)!}{k_1! (2\xi_{n,\ell} + 1)_{k_2} \Gamma(2\xi_{n,\ell} + k_1 + k_2 + 2L_1 + 2)!} \right]^{-\frac{1}{2}},
\]

\[
\tilde{\xi}_{n,\ell} = \sqrt{\frac{2\mu D_0}{a^2 h^2} + \ell(\ell + 1)d_0 - \frac{2\mu \xi_{n,\ell}^{(i)}}{a^2 h^2}},
\]

\[
L_1 = \frac{1}{2} + \sqrt{1 + \frac{2\mu D_0 \xi_{n,\ell}^{(i)}}{h^2} + \ell(\ell + 1)d_2},
\]

\[
d_0 = \frac{\bar{\lambda}}{2} + \frac{(1-\lambda) \xi_{n,\ell}^{(i)}}{\alpha},
\]

\[
d_1 = \lambda + \frac{(1-\lambda) \xi_{n,\ell}^{(i)}}{\alpha},
\]

\[
d_2 = \lambda + \frac{(1-\lambda) \xi_{n,\ell}^{(i)}}{\alpha},
\]

\[
d_3 = \frac{\xi_{n,\ell}^{(i)}}{\alpha^2 h^4} \frac{D_0}{\bar{\lambda}} + \ell(\ell + 1)\left(d_2 - d_1\right),
\]

\[
d_4 = D_0 + \left(\ell + 1\right)\frac{\bar{\lambda}^2}{\alpha^2 h^2} + \frac{2\mu \xi_{n,\ell}^{(i)}}{2\mu}.
\]

\[
\epsilon_{n,\ell}^{(i)} = \frac{1}{\bar{\alpha}} \left[ 3 - 3u + u^2 + (2u - 6)s_e + (u + 3) s_e^2 \right],
\]

\[
\epsilon_{n,\ell}^{(i)} = \frac{2}{u} s_e^2 (1 - s_e^2) \left[(3 + u)s_e + 2u - 3\right],
\]

\[
\epsilon_{n,\ell}^{(i)} = -\frac{1}{s_e^2} (1 - s_e^2)^3 \left((3 + u)s_e + u - 3\right),
\]

\[
s_e = e^{-\mu}, \quad u = \alpha r_e.
\]

In absence of the centrifugal term, the coefficients \(\gamma_{0,k} \to 0 \) as \(\xi \to \infty\) for \(k \geq 3\) which coincides with the reference [26] and the corresponding energy is approximated to the Morse-oscillator. The DF potential is very close to the Morse potential in the regions \(r \approx r_e\) and \(r > r_e\). We also checked that \(\gamma_{0,k} \to 0\) as \(D_e, \xi \to \infty\) for \(k \geq 3\) and then the DF and Morse potentials are approximated in the region \(r \approx r_e\) by a shifted harmonic oscillator with frequency \(\frac{a^2 h^2 \gamma_{0,1}}{2\mu}\).

1. Expectation values and average energy

The expectation of \(x^k\) with respect to a normalized time-dependent state \(\psi(x, t)\) is defined by

\[
\langle x^k \rangle^{(d)} = \int x^k \psi^*(x, t) \psi(x, t) \, dx,
\]

then

\[
\begin{align*}
\langle x \rangle^{(i)} &= L(T) \langle r \rangle^{(i)} + x_0 \beta, \\
\langle x^2 \rangle^{(d)} &= L(T)^2 \langle r^2 \rangle^{(i)} + 2x_0 \beta L(T) \langle r \rangle^{(i)} + x_0^2 \beta^2
\end{align*}
\]
where \( r_k^{(i)} = \int_0^\infty r^k |Q(r)|^2 dr \) are expectation values of \( r^k \) with respect to the corresponding TI state \( Q \). Then standard deviation of \( x \) is defined by

\[
\Delta x^{(d)} = \sqrt{\left[Z_x^{(d)} - (x^{(d)})^2\right]} = L(T) \sqrt{(r_x^{(i)}) - [(r_x^{(i)})]^2}
\]

The average energy of a normalized time-dependent state \( \psi(x, t) \) is found to be \([49, 50, 76–80]\),

\[
\langle \hat{E}\rangle_{n, \ell} = \int \psi^*(x, t) \frac{\partial \psi(x, t)}{\partial t} \, dx,
\]

\[
= \epsilon^{(i)} + \frac{\mu_x^2}{2 \hbar} \left[ \beta^2 - (L\bar{L} - \bar{L}^2) \right] \frac{\langle r_x^{(i)} \rangle}{x_0} + 2(L\bar{\beta} - \bar{L}\beta) \frac{\langle r_x^{(i)} \rangle}{x_0} - \hbar t_0 \bar{L} \frac{\langle r_x^{(i)} \rangle}{x_0} - \frac{\hbar \beta}{x_0 \mu_x^2} \bar{L} \frac{\langle r_x^{(i)} \rangle}{x_0} \tag{22}
\]

Then the expectation of \( x \) and \( x^2 \) with respect to the state \( \psi_{n, \ell}(x) \) is defined by

\[
\langle x \rangle_{n, \ell} = \frac{\langle N_n \rangle L^2}{\alpha(x_0^2 + 2)} \sum_{k=0}^{2n} \frac{2}{(k+2)!} B_{k+2, 2}
\times \left( c_0(n), 2cl_1(n), \ldots, (k+1)l_{c_k(n)} \right) I'_{n, \ell} + x_0 \beta \beta \alpha
\]

\[
\langle x^2 \rangle_{n, \ell} = \frac{\langle N_n \rangle L^2}{\alpha^2(x_0^2 + 2)} \sum_{k=0}^{2n} \frac{2}{(k+2)!} B_{k+2, 2}
\times \left( c_0(n), 2cl_1(n), \ldots, (k+1)l_{c_k(n)} \right) I''_{n, \ell} + x_0^2 \beta^2 \alpha
\]

where

\[
\chi'_{n, \ell} = \frac{2(L\bar{\beta} - \bar{L}\beta)}{x_0 \alpha} \sum_{k=0}^{2n} \frac{2}{(k+2)!} B_{k+2, 2}
\times \left( c_0(n), 2cl_1(n), \ldots, (k+1)l_{c_k(n)} \right) I'_{n, \ell}
\]

\[
\chi''_{n, \ell} = \frac{(L\bar{L} - \bar{L}^2)}{x_0 \alpha^2} \sum_{k=0}^{2n} \frac{2}{(k+2)!} B_{k+2, 2}
\times \left( c_0(n), 2cl_1(n), \ldots, (k+1)l_{c_k(n)} \right) I''_{n, \ell}
\]

The average energy of time-dependent potential (7) can be expressed as

\[
\langle \hat{E}\rangle_{n, \ell} = \epsilon^{(i)} + \frac{\mu_x^2}{2 \hbar} \left[ \beta^2 + \chi'_{n, \ell} + \chi''_{n, \ell} + \frac{\hbar t_0 \bar{L}}{x_0 \mu_x^2} \right]
\]

\[
\tag{25}
\]

where

\[
B(a, b) = \frac{\Gamma(a) \Gamma(b)}{\Gamma(a+b)} \text{ is the usual Beta function, } \Psi(x) = \frac{\Gamma'(x)}{\Gamma(x)} \text{ is the digamma function. Furthermore,}
\]

\[
B_{m, j}(x_1, x_2, \ldots, x_{m-j+1})
\]

\[
= \sum_{n=0}^{m!} \frac{j_1!j_2! \cdots (x_{m-j+1})!}{(m-j+1)!}
\]

\[
\times \left( \frac{x_1}{2!} \right)^{j_1} \left( \frac{x_2}{2!} \right)^{j_2} \cdots \left( \frac{x_{m-j+1}}{(m-j+1)!} \right)^{j_{m-j+1}} \tag{27}
\]

is the Bell polynomial, where \( \pi(m, j) \) denotes the set of partitions, such that \( j_1 + j_2 + \cdots + j_{m-j+1} = j \), \( j_1 + j_2 + \cdots + (m-j+1) = m \), and \( c_k(n) = \frac{(-1)^{n-k}k!(2x_0\beta)^{n-k}}{k!(\bar{L}^n+2\bar{L})}, \) if \( k \leq n \), while \( c_k(n) = 0 \), if \( k > n \).

In particular, for \( L = \kappa \), a constant, one obtains

\[
\langle \hat{E}\rangle_{n, \ell} = \frac{\epsilon^{(i)} + \mu_x^2}{2 \hbar} \left[ \beta^2 \right] + \frac{2\kappa \beta}{x_0 \alpha} \left( \frac{N_n}{\kappa} \right)^2 \sum_{k=0}^{2n} \frac{2}{(k+2)!} B_{k+2, 2}
\times \left( c_0(n), 2cl_1(n), \ldots, (k+1)l_{c_k(n)} \right) I'_{n, \ell}
\]

\[
\tag{28}
\]

2.2 Time-correlation function, disequilibrium and quantum similarity

The time-correlation function between states \( \psi_{n_1, \ell_1} \) and \( \psi_{n_2, \ell_2} \) can be defined as \([80–82]\),

\[
C^{(d)}(n_1, \ell_1, n_2, \ell_2) = \int_0^\infty \psi_{n_1, \ell_1}(x, t_1) \psi_{n_2, \ell_2}(x, t_2) dx
\]

\[
\tag{29}
\]

where \((x_0 \beta_{12}, \infty)\) is the common domain of overlap integral of moving boundary solutions, and \( \beta_{12} = \max[\beta(T_1), \beta(T_2)] \). The quantity \( C^{(d)}(n_1, \ell_1, n_2, \ell_2) \) is called the cross-correlation function of \( \psi_{n_1, \ell_1}(x, t_1) \) and \( \psi_{n_2, \ell_2}(x, t_2) \). Similarly, \( C^{(d)}(n, \ell, n, \ell) \) is called the auto-correlation function of \( \psi_{n, \ell}(x, t) \) at different time domains \( t_1 = t_2 = t \) but at the same time \( C^{(d)}(n, \ell, t_1, t_1) = 1 \). The quantum similarity measure between two states with densities \( \rho_{n_1, \ell_1}(x, t) \) and \( \rho_{n_2, \ell_2}(x, t) \) can be defined as

\[
\mathcal{M}^{(d)}(n_1, \ell_1, n_2, \ell_2) = \int_0^\infty \rho_{n_1, \ell_1}(x, t) \rho_{n_2, \ell_2}(x, t) dx
\]

\[
\tag{30}
\]
Table 1  Set of parameters for diatomic molecules [39] considered in this work

| Molecule | $D_e$(eV) | $r_e$(Å) | $\alpha$(Å$^{-1}$) | $\mu$(amu) | Molecule | $D_e$(eV) | $r_e$(Å) | $\alpha$(Å$^{-1}$) | $\mu$(amu) |
|----------|-----------|----------|---------------------|-----------|----------|-----------|----------|---------------------|-----------|
| H$_2$    | 4.7446    | 0.7416   | 1.9426              | 0.50391   | LiH      | 2.5152672118 | 1.5956 | 1.1280              | 0.8801221 |
| HCl      | 4.619030905 | 1.2746 | 1.8677              | 0.9801045 | ScH      | 2.25      | 1.776  | 1.41113              | 0.986040  |
| TiH      | 2.05      | 1.781    | 1.32408             | 0.987371  | VH       | 2.33      | 1.719  | 1.44370              | 0.988005  |
| CrH      | 2.13      | 1.694    | 1.52179             | 0.988976  | CO       | 11.2256  | 1.1283 | 2.2994              | 6.8606719 |

Fig. 1  Plot of density functions of molecules in TD system for $x_0 = 1$ Å, $L(T) = \sqrt{1.5T^4 + 2.5T + 1}$, $\beta(T) = \sin^2(2\pi T/3)$. For more details, see text

The quantity $M_{(n,\ell), (n,\ell)}(t)$ represents disequilibrium of a given state, $\psi_{n,\ell}(x, t)$, and we denote it as $D^{(d)}_{(n,\ell)}(t)$. It is also called self-similarity [83,84] of a state. The disequilibrium $D^{(d)}_{(n,\ell)}(t)$ is defined by,

$$D^{(d)}_{(n,\ell)}(t) = \frac{\alpha [N_{n,\ell}]^4}{L(T)} \sum_{k=0}^{4n} 243k+4.4 \left[ c^{(n)}_0, 2! c^{(n)}_1, \ldots, (k+1)! c^{(n)}_k \right] \Gamma(4\tilde{\epsilon}_{n,\ell} + k + 4L_1 + 1) \Gamma(4\tilde{\epsilon}_{n,\ell} + k) \frac{\Gamma(4\tilde{\epsilon}_{n,\ell} + k + 4L_1 + 1)}{(k+4)!(4L_1 + 1)}.$$  \hspace{1cm} (31)

On the other hand, $D^{(i)}_{(n,\ell)}$ represents the disequilibrium of a certain state, $Q_{n,\ell}(r)$ and one obtains $D^{(d)}_{(n,\ell)}(t) = D^{(i)}_{(n,\ell)}/L(T)$. Then the quantum similarity index (QSI) between two states of a time-dependent system is defined by,

$$S^{(d)}_{(n_1,\ell_1),(n_2,\ell_2)}(t) = \frac{M^{(d)}_{(n_1,\ell_1),(n_2,\ell_2)}(t)}{\sqrt{D^{(d)}_{(n_1,\ell_1)}(t)D^{(d)}_{(n_2,\ell_2)}(t)}}.$$  \hspace{1cm} (32)

The quantum similarity measure (QSM), $M^{(d)}_{(n_1,\ell_1),(n_2,\ell_2)}(t)$, is then written as [50],

$$M^{(d)}_{(n_1,\ell_1),(n_2,\ell_2)}(t) = \frac{M^{(i)}_{(n_1,\ell_1),(n_2,\ell_2)}}{L(T)},$$

where $M^{(i)}_{(n_1,\ell_1),(n_2,\ell_2)} = \int_0^\infty \left[ |Q_{n_1,\ell_1}(q)|^2 |Q_{n_2,\ell_2}(q)|^2 \right] dq$, is the QSM of respective TI quantum system (4), and thus one finally obtains, $S^{(d)}_{(n_1,\ell_1),(n_2,\ell_2)}(t)$.
Fig. 2 Analogous to Fig. 1, with $L(T) = 1, \beta(T) = 0.5T^2$

Fig. 3 Left four panels: H$_2$, HCl, LiH and ScH; right four panels: TiH, CrH, VH and CO. Panels A, C, E, G show motion of peak points of ground state of TD system, while B, D, F, H show peak values of the state. For A, C, E, and G, $L(T) = \sqrt{1.5T^2 + 2.5T + 1}, \beta(T) = \sin^2(2\pi T/3)$, and for B, D, F, and H, $L(T) = 1, \beta(T) = 0.5T^2, x_0 = 1\text{Å}, \ell = 2$. 
Table 2  Radial expectation values of diatomic molecules

\[(n, \ell) \quad H_2 \quad LiH \quad HCl \quad ScH \quad TiH \quad VH \quad CrH \quad CO\]

\[
\begin{array}{ccccccccc}
(n, \ell) & H_2 & LiH & HCl & ScH & TiH & VH & CrH & CO \\
\hline
(0,0) & 0.769726 & 1.622835 & 1.292479 & 1.801313 & 1.807815 & 1.743898 & 1.719886 & 1.132518 \\
(0,1) & 0.770410 & 1.623088 & 1.292578 & 1.801445 & 1.807977 & 1.744032 & 1.720025 & 1.132523 \\
(0,2) & 0.771779 & 1.623593 & 1.292776 & 1.801709 & 1.808300 & 1.744300 & 1.720302 & 1.132534 \\
(0,3) & 0.773836 & 1.624351 & 1.293073 & 1.802105 & 1.808785 & 1.744702 & 1.720718 & 1.132547 \\
(1,0) & 0.828688 & 1.678833 & 1.329420 & 1.853758 & 1.863333 & 1.795492 & 1.773734 & 1.141034 \\
(1,1) & 0.829442 & 1.679100 & 1.329525 & 1.853899 & 1.863506 & 1.795636 & 1.773883 & 1.141050 \\
(1,2) & 0.830952 & 1.679634 & 1.329736 & 1.854182 & 1.863851 & 1.795923 & 1.774182 & 1.141068 \\
(1,3) & 0.833222 & 1.680436 & 1.330053 & 1.854606 & 1.864370 & 1.796354 & 1.774631 & 1.141086 \\
(2,0) & 0.904769 & 1.746916 & 1.372033 & 1.913900 & 1.927645 & 1.854751 & 1.835452 & 1.150440 \\
(2,1) & 0.905605 & 1.747199 & 1.372146 & 1.914000 & 1.927830 & 1.854905 & 1.835614 & 1.150446 \\
(2,2) & 0.907281 & 1.747765 & 1.372371 & 1.914300 & 1.928201 & 1.855213 & 1.835938 & 1.150458 \\
(2,3) & 0.909802 & 1.748614 & 1.372710 & 1.914800 & 1.928757 & 1.855676 & 1.836423 & 1.150474 \\
\end{array}
\]

\[
\begin{array}{ccccccccc}
(n, \ell) & H_2 & LiH & HCl & ScH & TiH & VH & CrH & CO \\
\hline
(0,0) & 0.598706 & 2.645376 & 1.675913 & 3.255103 & 3.279612 & 3.051118 & 2.967980 & 1.283656 \\
(0,1) & 0.599770 & 2.646200 & 1.676170 & 3.255581 & 3.280199 & 3.051588 & 2.968459 & 1.283668 \\
(0,2) & 0.601903 & 2.647849 & 1.676684 & 3.256537 & 3.281373 & 3.052527 & 2.969416 & 1.283693 \\
(0,3) & 0.605117 & 2.650325 & 1.677456 & 3.257972 & 3.283136 & 3.053937 & 2.970854 & 1.283730 \\
(1,0) & 0.705961 & 2.854365 & 1.783851 & 3.468080 & 3.506842 & 3.254120 & 3.176615 & 1.305151 \\
(1,1) & 0.707246 & 2.855275 & 1.784134 & 3.468610 & 3.507495 & 3.254642 & 3.177153 & 1.305163 \\
(1,2) & 0.709823 & 2.857094 & 1.784703 & 3.469672 & 3.508800 & 3.255686 & 3.178227 & 1.305189 \\
(1,3) & 0.713706 & 2.859827 & 1.785555 & 3.471266 & 3.510759 & 3.257253 & 3.179841 & 1.305227 \\
(2,0) & 0.850692 & 3.111947 & 1.910435 & 3.774197 & 3.916393 & 3.420849 & 3.428859 & 1.328872 \\
(2,1) & 0.852267 & 3.112957 & 1.910750 & 3.775646 & 3.922222 & 3.421455 & 3.428872 & 1.328872 \\
(2,2) & 0.855427 & 3.114978 & 1.911380 & 3.778505 & 3.933388 & 3.422667 & 3.428899 & 1.328899 \\
(2,3) & 0.860191 & 3.118013 & 1.912326 & 3.720284 & 3.779294 & 3.495139 & 3.424488 & 1.328938 \\
\end{array}
\]

![Fig. 4](image-url) Average energy (eV) of molecules in TD system. In A, B: \( L(T) = 1, \beta(T) = \sin^2(2\pi T) \), C, D: \( \beta(T) = \sqrt{0.5T^2 - 0.5T + 1}, L(T) = T^2 + 1 \). Parameters are: \( x_0 = 0.01\ \text{Å}, cT_0 = 250000\ \text{Å} \).
Fig. 5 Plot of correlation functions. Left column real part of $C_{0,1}(t,0)$, middle column imaginary part of $C_{0,1}(t,0)$ and right column real vs imaginary parts of $C_{0,1}(t,0)$. The red, blue, black, green, magenta, orange, cyan lines represent LiH, HCl, ScH, TiH, VH, CrH and CO molecules, respectively. This figure is defined for $c t_0 = 250000 \text{Å}$, $x_0 = 0.01 \text{Å}$, $\beta = \sin^2(2\pi T/3)$, $L(T) = \sqrt{1.5T^2 + 2.5T + 1}$

3 Results and discussions

The molecular parameters $D_e$, $r_e$ and $\mu$ are taken from ref. [39]. They are listed in Table 1. The following conversion factors have been used throughout the whole work: $1 \text{amu} = 931.494028 \text{ MeV}/c^2$, $1 \text{ cm}^{-1} = 1.239841875 \times 10^{-4} \text{ eV}$, $c \hbar = 1973.29 \text{ eV}\text{Å}$, where $c$ is the speed of light.

In Figs. 1 and 2, we have plotted density functions of the diatomic molecules of above table, with moving boundary conditions. For the first figure, we have considered $L(T) = \sqrt{1.5T^2 + 2.5T + 1}$, $\beta(T) =$
$\sin^2(2\pi T/3)$, while for the latter one, we employ $L(T) = 1$, $\beta(T) = 0.5 T^2$, respectively. In both cases, $x_0 = 1\text{Å}$. It may be mentioned that the density plots in Figs. 1 and 2 give the resemblance of soliton solitary waves and each density has a peak. The peak point, $x = x_{0,\ell}$, of the density function, $|\psi_{0,\ell}(x, t)|^2$, is obtained from the conditions, $\left[\frac{\partial |\psi_{0,\ell}(x, t)|^2}{\partial x}\right]_{x=x_{0,\ell}} = 0$, $\left[\frac{\partial^2 |\psi_{0,\ell}(x, t)|^2}{\partial x^2}\right]_{x=x_{0,\ell}} < 0$. Then, the peak of the density function moves along the curve: $x_{0,\ell} = x_0 \beta(T) + \frac{L(T)}{\alpha} \ln \left[ L_1 + \frac{\tilde{\varepsilon}_0 T}{\tilde{\varepsilon}_{0,\ell}} \right]$, and the corresponding peak value is defined by: $|\psi_{0,\ell}(x_{0,\ell}, t)|^2 = \frac{\alpha^2 N_0^2 \tilde{\varepsilon}_0^2 L_1^4 (L(T)/(\tilde{\varepsilon}_0 T + L_1)^3)}{L(T)/(\tilde{\varepsilon}_0 T + L_1)^3 + 2L_1}$. If $L(T)$ is a constant, then the peak value is a constant.

The motions of peak points of ground state of all molecules are shown in (A),(C),(E),(G) panels of Fig. 3, and corresponding peak values are shown in panels (B),(D),(F),(H). Moreover, (A)-(D) provide results for H2, LiH, HCl, ScH, whereas (E)-(H) give the same for TiH, VH, CrH and CO. The segments (A),(C),(E),(G) are generated by considering $L(T) = \sqrt{1 - 0.5 T + 0.5 T^2}$, $L_3(T) = 1 + T^2$. Other parameters are: $x_0 = 0.01\text{Å}$, $c_0 = 250000\text{Å}$, $n = 0$, $\ell = 1$.
tion are qualitatively similar, but there are numerical differences.

In Table 2 now, we have produced the calculated expectation values of $r$ and $r^2$ of all the diatomic molecules, in TI quantum system in Å and Å$^2$ units, respectively, for $n = 0, 1, 2$, $\ell = 0, 1, 2, 3$. These cannot be directly compared with reference results, as the literature values are absent. However, it is worth mentioning that the calculated eigenvalues have been checked and compared with other existing results earlier, which shows excellent agreement. These comparisons have been presented earlier [42] to demonstrate the success and efficacy of present method, and hence not repeated here.

It is worth mentioning that in absence of the moving boundary, the DF potential generally offers bound states with real energies, called ro-vibrational energies. There is a maximum possible quantum number $\ell$ (or $n$) for a fixed $n$ (or $\ell$) for which energies are non-negative. But in presence of the moving boundary condition, the average energies are complex, in general. For a particular scaling factor $L = \text{constant}$, we obtain real average energies for a given quantum number $n$ and $\ell$. Now, one can find a maximum possible quantum number $\ell$ (or $n$) for a fixed $n$ (or $\ell$) for which energies are real and non-negative. In Fig. 4, we have plotted the average energy of eight diatomic molecules in eV units, along two different curves. In panels (A), (B), we have considered periodic moving boundary condition and in (C), (D) parabolic moving boundary condition have been used. The panels (A), (B), (C), (D) provide average energy variations of $H_2$, LiH, HCl, Sch, TiH, VH and CrH, CO molecules, respectively. Note that (A), (C) offers these plots for ground state, while the other two panels (B), (D) correspond to states having radial and angular quantum numbers $n_r = 0$ and $\ell = 2$. The similarity between (A), (B) and (C), (D) is quite visible. The average energies of $H_2$ and LiH at $t = 0$ are: 0.3895eV and 0.0742eV, respectively, but their ro-vibrational energies in absence of moving boundary condition are: 0.349980221eV and 0.103334650eV [42] for $n_r = \ell = 0$. Under the choice of scale factor $L$ and moving boundary condition, $\psi(x_0, \beta(T), t) = 0$, one can find average energy, and the corresponding average force acting on the boundary wall in a confined region. This method can be extended to time-dependent confined quantum systems as well.

Now the time-correlation function of two molecules is plotted in Fig. 5. In left and middle columns, we have

| $H_2$ | LiH | HCl | Sch | TiH | VH | CrH | CO |
|-------|-----|-----|-----|-----|----|-----|----|
| 1 | 0.0000000002297 | 0.00000000000017 | 0.00000000000010 | 0.00000000000000 | 1 | 1 | 1 |
| LiH | 1 | 0.0000000002297 | 0.00000000000017 | 0.00000000000010 | 0.00000000000000 | 1 | 1 | 1 |
| HCl | 0.00000000000010 | 0.00000000000017 | 0.00000000000010 | 0.00000000000000 | 1 | 1 | 1 | 1 |
| Sch | 0.00000000000010 | 0.00000000000017 | 0.00000000000010 | 0.00000000000000 | 1 | 1 | 1 | 1 |
| TiH | 0.00000000000010 | 0.00000000000017 | 0.00000000000010 | 0.00000000000000 | 1 | 1 | 1 | 1 |
| VH | 0.00000000000010 | 0.00000000000017 | 0.00000000000010 | 0.00000000000000 | 1 | 1 | 1 | 1 |
| CrH | 0.00000000000010 | 0.00000000000017 | 0.00000000000010 | 0.00000000000000 | 1 | 1 | 1 | 1 |
| CO | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
plotted the real and imaginary parts of time-correlation $C_{0,1}(t, 0)$. In the last column, we have shown the same in the complex plane of $(\text{Re} [C_{0,1}(t, 0)], \text{Im} [C_{0,1}(t, 0)])$. In the first row, we have compared the time-correlation function of $H_2$ with LiH, HCl, ScH, TiH, VH, CrH and CO, which are represented by red, blue, black, green, magenta, orange and cyan colours, respectively. The second row compares the same for LiH with HCl, ScH, TiH, VH, CrH and CO, which is represented by blue, black, green, magenta, orange and cyan lines, respectively. Similarly the last row compares this between CrH and CO. In this row, we have plotted $10^6 C_{0,1}(t, 0)$. From this figure, it is observed that the time-correlation of CO with other molecules is very small compared with other pairs.

As we stated earlier, quantum similarity is time dependent but quantum similarity index is time independent for a given potential [50]. We can see that the potential, Eq. (1) is dependent on parameters, $D_e, r_e, \alpha, \mu$. Therefore for two sets of parameters the potential has two values. Therefore, for two diatomic molecules, we observe that $M^{(d)}_{(n_1, \ell_1), (n_2, \ell_2)}(t) \neq M^{(i)}_{(n_1, \ell_1), (n_2, \ell_2)}/L(T)$. In this case, we follow the definition of Eq. (30) for quantum similarity, and for quantum similarity index, we follow the definition of Eq. (32). In Fig. 6, we plot the quantum disequilibrium of molecules with respect to $T$. The disequilibrium decreases as $T$ increases, and their qualitative features are similar even though their magnitude is different.

The black, blue and red colours represent (i) $\beta_1(T) = \sin(2\pi * T)^2$, $L_1(T) = \sqrt{1 - 0.25T + 0.25T^2}$; (ii)
Table 4  Range of time-dependent QSI of diatomic molecules

|     | \(H_2\) | LiH | HCl | ScH | TiH | VH | CrH | CO |
|-----|---------|-----|-----|-----|-----|----|-----|-----|
| \(j\) | \(a_{ij}\) | \(10^3 b_{ij}\) | \(a_{2j}\) | \(b_{2j}\) | \(a_{3j}\) | \(b_{3j}\) |
| LiH | 0.000002257154 | 0.000002297818 | 0.036554830676 | 0.36554830693 | 0.0018789325805 | 0.0018789325813 |
| HCl | 0.024038045899 | 0.024038045914 | 0.48172116834 | 0.481721168436 | 0.00002380209075 | 0.000023802090992 |
| ScH | 0.000000000161 | 0.000000000180 | 0.474482852606 | 0.474482852339 | 0.00010015365391 | 0.0001001536596 |
| TiH | 0.000000000294 | 0.000000000321 | 0.798822163132 | 0.798822164339 | 0.0002054037333 | 0.0002054037335 |
| VH | 0.000000000189 | 0.0000000002078 | 0.706149730366 | 0.706149730913 | 0.0010015363591 | 0.0010015363596 |
| CrH | 0.0000000005830 | 0.0000000006446 | 0.492923770764 | 0.492923771003 | 0.000084712753 | 0.000084712755 |
| CO | 0.492923770764 | 0.492923771003 | 0.0000084712753 | 0.0000084712755 | 0.113219084218 | 0.113219084320 |

\(\beta_2(T) = \sin(2\pi T)\), \(L_2(T) = 1\); (iii) \(\beta_3(T) = \sqrt{1 - 0.5T^2 + 0.5T^2}, L_3(T) = 1 + T^2\), having \(x_0 = 0.01\) Å, \(c_{t0} = 250000\) Å for the state characterized by quantum numbers, \(n = 0, \ell = 1\). If the scale factor \(L\) is constant, then disequilibrium remains constant. However, disequilibrium decreases (or increases) if \(L(T)\) increases (or decreases).

In Table 3, the QSI between two diatomic molecules at \(t = 0\) are given. Next, in Fig. 7, we plot the time-dependent QSI between two diatomic molecules. The interval \((a_{ij}, b_{ij})\) represents the range of QSI of \(i\)th and \(j\)th molecules, where \(i = 1, 2, 3, \cdots, 7\) represents \(H_2, \ LiH, \ HCl, \ ScH, \ TiH, \ VH, \ CrH\) and \(j = 1, 2, \cdots, 7\) refers to \(LiH, \ HCl, \ ScH, \ TiH, \ VH, \ CrH, \ CO\). Table 4 produces the calculated numerical values of \(a_{ij}\) and \(b_{ij}\). Note that close similarity of \(ScH\) and \(TiH\) as evidenced by the QSI values is reminiscent of our previous study [85] of these molecules in presence of a pseudo-harmonic potential. Here, we investigated QSI among 19 molecules in presence of pseudo-harmonic and its iso-spectral potentials. Here also, it is found that: (i) QSI between \(ScH\) and \(TiH\) is maximum, (ii) CO molecule shows maximum dissimilarity with other molecules, such as, \(H_2, \ LiH, \ HCl, \ ScH, \ TiH, \ VH, \ CrH, \) which is amply clear from Table 3, (iii) four species, namely \(ScH, \ TiH, \ VH\) and \(CrH\), are quite similar (iv)

The QSI between \(H_2\) and \(ScH\) is minimum which is in conformity with our previous study [85]. The time-dependent QSI satisfies all these properties (i)-(iv) in a time-dependent quantum system with moving boundary condition. The time-dependent QSI between two molecules changes with respect to time in a very short range, which confirms that QSI is a fixed number up to a certain round of approximation [50] and it lies between 0 to 1.

### 4 Conclusion

Exact solutions of time-dependent Schrödinger equation is obtained in presence of Deng-Fan potential using a simple novel approximation of the centrifugal term. The time-dependent average energy is defined for an arbitrary moving boundary condition and it is expressed in terms of scale factors \(x_0, t_0\) and \(L\). These are performed for eight representative molecules, namely, \(H_2, \ LiH, \ HCl, \ ScH, \ TiH, \ VH, \ CrH, \ CO\). The boundary moves along two different curves. The motion of the peak of density function has been shown analytically for arbitrary moving moving boundary condition for ground states of some diatomic molecules; the corresponding peak values are defined analytically.
The numerical peak values are defined for parabolic and periodic moving boundary condition. The numerical values of time-dependent QSI between pairs of diatomic molecules are presented in detail. The densities of solitary wave functions of ScH, TiH, VH, CrH molecules are quite similar. Moreover, they are similar with respect to time-dependent average position, average energy, disequilibrium, quantum similarity as well as QSI.

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Data Availability All data generated or analysed during this study are included in this article.

Conflict of interest The authors declare that they have no conflict of interest.

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