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Dynamics of Particle in a Box in Time Varying Potential Due to Chirped Laser Pulse

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Abstract

We describe a computational method for simulating the time dependent quantum mechanical system interacting with external field. In this method the Schrödinger equation is solved by expanding the wave function in the basis set of unperturbed Hamiltonian. The expansion yields a set of coupled first order differential equation. For expansion coefficients, the coupled channel method is applied to a particle in a box interacting with external field in the form of chirped laser pulse. The pulse shape is taken as Gaussian. We study the effect of different pulse parameters *i.e.* chirp rate, intensity, center frequency, box length and laser duration on the dynamics of the particle. Many interesting results are obtained and explained.

1. Introduction

Quantum mechanics [1,2] is the fundamental base for several branches in Physics and particle in a box is one of the fundamental problems of quantum mechanics. In this paper, we have studied dynamics of a particle in a box in time varying external field/potential. This time varying field is achieved using a chirped laser pulse. Wang and Champagne [3] have studied the interaction of Gaussian laser pulse with the particle in a box. In their study they found that by using laser centre frequency to be resonant with the transition between first two states *i.e.* $n = 1$ and $n = 2$, transition probability of $n = 2$ state is appreciable and all other higher state have non zero but negligible probability. Here, we are presenting numerical simulation of the system. We numerically solve the coupled differential equations obtained for a particle in a box, in the presence of a chirped laser pulse. It is shown that high-efficiency population transfer is possible for several values of chirp rate and box length. We also explore the dependence of population transfer on chirp rate. The results indicate that we can have large transition probabilities for higher states also with the help of chirped laser pulse.

With the development in laser technology [4-6] in recent years, various techniques have been developed to modulate and even shape the laser pulse. The most exploited feature of modulated pulse is the chirp which describes the variation of carrier frequency with time. If the frequency in-

creases with the time, the pulse is positively chirped and if the frequency decreases with time, it is negatively chirped. Ruhman and Kosloff [7] used negatively chirped pulse to achieve large amplitude of vibrational motion in higher vibrational states of the ground electronic surface of CsI through an effective intra pulse pump dump mechanism. Cao *et al.* [8] have studied that a positively chirped pulse is very efficient in population inversion. So both positive and negative chirps are important and can be used as per requirement of the problem or the system. The selection also depends on the system with which the laser pulse is interacting and other parameters of pulse e.g. intensity, center frequency, pulse width etc. No work for such type of problem has been published earlier. Recently coherent control for box potential with laser fields has been studied by Imre F. Barna and PéterDombi [9].

In this paper we have used numerical method and computer simulation to express all results. In Section 2, we have described a general coupled channel method to solve the Schrödinger equation under time dependent perturbation condition. The Schrödinger equation is reduced to a set of first order coupled differential equations which are solved using efficient and commonly used fourth order Runge-Kutta method. Section 3 briefly describe particle in a box and its interaction with chirped laser pulse. We apply the coupled channel method to find the solution. In Section 4, we briefly describe the computer simulation work. Finally in Section 5, we describe the numerical results for the

transition probabilities for different states as a function of time, chirp rate, box length and laser center frequency. Particularly, effect of linear chirp is examined in detail. In Section 6, we conclude the paper.

2. The Coupled Channel Method

The coupled channel method [10,11] is used to solve the time dependent Schrödinger equation. Consider a quantum mechanical system having unperturbed Hamiltonian $\hat{H}_0$ for a eigen state $|\chi_n\rangle$ with eigen energy values E_n which satisfy the equation

$$\hat{H}_0|\chi_n\rangle = E_n|\chi_n\rangle \tag{1}$$

Here $|\chi_n\rangle$ forms a complete orthogonal set of eigen vectors *i.e.*

$$\sum \langle \chi_n | \chi_n \rangle = 1, \ |\chi_n\rangle\langle\chi_n| = \delta_{mn} \tag{2}$$

Considering the wave function as

$$|\psi(t)\rangle = \sum_n a_n(0)\exp(-iE_nt/\hbar)|\chi_n\rangle \tag{3}$$

Without perturbation wave function will have usual time dependence but coefficient a_n is independent of time. Let us consider that perturbation is turned on instantaneously at $t = 0$. Then the full Hamiltonian will be described as

$$\hat{H} = \hat{H}_0 + V(t) \tag{4}$$

$$\hat{H}|\chi_n\rangle = \left(\hat{H}_0 + V(t)\right)|\chi_n\rangle \tag{5}$$

$V(t)$ is the perturbation part (which is a function of time) having condition

$$\begin{aligned} V(t) &= 0 & t \le 0 \\ V(t) &\ne 0 & t \ge 0 \end{aligned} \tag{6}$$

Now the time dependent Schrödinger equation is (as explained in Section 5, box units are used throughout the paper)

$$i\hbar \frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle \tag{7}$$

The solution of "(7)" can be written as

$$|\psi(t)\rangle = \sum_n a_n(t)\exp(-iE_nt/\hbar)|\chi_n\rangle \tag{8}$$

Here a_n (probability amplitudes) acquire time dependence. In the absence of external perturbation, if system is in one of the eigen state of $\hat{H}_0$, then it will remain in that state forever. However by the presence of a small perturbation, the system makes transition between its unperturbed eigen states. So with the perturbation, the probability of finding the system in n^{th} state at any time t will vary with time and $P_n(t)$ is given by

$$P_n(t) = |a_n(t)|^2 \tag{9}$$

Using "(4)" in "(7)"

$$i\hbar \frac{\partial|\psi(t)\rangle}{\partial t} = \left(\hat{H}_0 + V(t)\right)|\psi(t)\rangle \tag{10}$$

Using "(1)" and "(8)" in "(10)", we get the following equation

$$\sum_n \left\{ i\hbar \frac{\partial a_n(t)}{\partial t}\exp(-iE_nt/\hbar) + E_na_n(t)\exp(-iE_nt/\hbar) \right\}|\chi_n\rangle$$
$$= \sum_n a_n(t)\exp(-iE_nt/\hbar)E_n|\chi_n\rangle + \sum_n a_n(t)\exp(-iE_nt/\hbar)V|\chi_n\rangle \tag{11}$$

Or

$$\sum_n i\hbar \frac{\partial a_n(t)}{\partial t}\exp(-iE_nt/\hbar)|\chi_n\rangle = \sum_n a_n(t)\exp(-iE_nt/\hbar)V|\chi_n\rangle \tag{12}$$

Operating it with $|\chi_k\rangle$ from left, we get

$$\sum_n i\hbar \frac{\partial a_n(t)}{\partial t}\exp(-iE_nt/\hbar)\langle\chi_k|\chi_n\rangle = \sum_n a_n(t)\exp(-iE_nt/\hbar)\langle\chi_k|V|\chi_n\rangle \tag{13}$$

$$i\hbar \frac{\partial a_k(t)}{\partial t}\exp(-iE_nt/\hbar) = \sum_n a_n(t)\exp(-iE_nt/\hbar)\langle\chi_k|V|\chi_n\rangle \tag{14}$$

Let the transition matrix element be

$$V_{kn} = \langle\chi_k|V|\chi_n\rangle \tag{15}$$

The transition matrix element V_{kn} may be either zero or non-zero depending upon the selection rules. Considering transition frequency as $\omega_{kn} = (E_k - E_n)\hbar$, Equation

(14) will become

$$i\hbar\frac{\partial a_k(t)}{\partial t} = \sum_n a_n(t)\exp(i\omega_{kn}t)V_{kn} \qquad (16)$$

Thus matrix differential equation for co-efficients a_n is

$$i\hbar\begin{pmatrix}\dot{a}_1\\\dot{a}_2\\\cdot\\\cdot\\\dot{a}_n\end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}\exp(i\omega_{12}t) & \cdot & \cdot \\ V_{21}\exp(i\omega_{21}t) & V_{22} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & V_{nn}\end{pmatrix}\begin{pmatrix}a_1\\a_2\\\cdot\\\cdot\\a_n\end{pmatrix} \qquad (17)$$

And by solving this set of coupled differential equations we get value of $a_n(t)$ for different states and hence probability of finding the system in any particular state at any time t. We can write

$$a_n(t) = R_n(t) + iI_n(t) \qquad (18)$$

where $R_n(t)$ and $I_n(t)$ are real and imaginary part of $a_n(t)$ respectively. Using (18) in (16) we can have

$$i\hbar\left(\frac{\partial R_k(t)}{\partial t} + i\frac{\partial I_k(t)}{\partial t}\right) =$$
$$\sum_n \left(R_n(t) + iI_n(t)\right)\left(\cos(\omega_{kn}t) + i\sin(\omega_{kn}t)\right)V_{kn} \qquad (19)$$

Separating real and imaginary parts of $a_n(t)$ we get following equations

$$\hbar\frac{\partial R_k(t)}{\partial t} = \sum_n R_n(t)\sin(\omega_{kn}t)V_{kn} + I_n(t)\cos(\omega_{kn}t)V_{kn} \qquad (20)$$

$$\hbar\frac{\partial I_k(t)}{\partial t} = -\sum_n R_n(t)\cos(\omega_{kn}t)V_{kn} + I_n(t)\sin(\omega_{kn}t)V_{kn} \qquad (21)$$

Equation (20) and (21) can be solved by using numerical methods e.g. Runge-Kutta Method.

3. Particle in a Box in Chirped Laser Field

Consider a particle *i.e.* electron in a deep potential well from which it cannot escape and loses no energy when it collide with walls. So the potential is defined as

$$V(x) = 0 \qquad 0 < x \leq L$$
$$V(x) = \infty \qquad x < 0, \; x > L \qquad (22)$$

Now the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x) \qquad (23)$$

By solving this equation, the unperturbed eigen function and the eigen energy value are

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(nx/L) \qquad (24)$$

and

$$E_n = \hbar^2\pi^2 n^2 \big/ (2mL^2) \qquad (25)$$

where L is the length of the box and $n = 1, 2, 3, \cdots$, and $n \neq 0$ as it will give probability of finding the particle everywhere equal to zero, which is not possible. Consider that the system is interacted with chirped laser pulse [12]. Here the laser field is defined as

$$E(t) = E_0\sin^2(\pi t/\tau)\cos(\omega_0 + \beta t)t \qquad (26)$$

Here E_0, τ, ω_0 and β are the amplitude, laser duration, laser center frequency and the chirp rate respectively. The laser interaction with the particle (*i.e.* electron) is defined as

$$V(x,t) = e.E(t)(x - L/2) \qquad (27)$$

Here 'e' is electron charge and zero point potential is chosen at $L/2$. Now the transition matrix V_{kn} can be written as

$$V_{kn}(t) = \int eE(t)\psi_k^*(x)(x - L/2)\psi_n(x)\,dx$$
$$= eE(t)\int \psi_k^*(x)(x - L/2)\psi_n(x)\,dx \qquad (28)$$
$$= eE(t)D_{kn}$$

where

$D_{kn} = 0$ if $k = n$ or $k + n$ is even,

$D_{nk} = -8Lkn\big/\pi^2\left(k^2 - n^2\right)^2$ if $k + n$ is odd

Using this transition matrix V_{kn} in Equation (20) and (21), we can find excitation/transition probability of any state at any time t under chirped laser field. By using linear chirp, we will get some exciting new results which is unexpected by simple laser pulse. These are described in the results section.

4. Computational Analysis

The determination of coefficients $a_n(t)$ of different states allows us to calculate the transition probability for various laser pulse parameters. For the present calculations, we have studied the system with $n = 10$ levels. Further, we have checked the convergence by variation in number of levels, and have obtained excellent convergence with $n = 10$ levels.

For making the calculations traceable we have separated the real and imaginary parts of the coefficients $a_n(t)$ [see (18-21)]. Thus we obtain 20 real coupled differential equations to be solved. Any time propagator scheme can be used to solve these equations. For solving these equations we have used the efficient fourth order Runge-Kutta method by assuming that the system is initially in the ground state.

In next section, we discuss the results thus obtained.

5. Results

It is worth mentioning, here, that we have used the box units throughout the paper. In this system of unit, the unit of mass is electron mass (m_e), unit of length is 10^{-10} *m*, unit of time is 1.75×10^{-17} *s*, unit of electric field is 3.75×10^{11} *V/m* and unit of energy is ground state energy of electron in box of length 10^{-10} *m i.e.* 37.5 *eV* . Consider that initially the particle is in ground state *i.e.* $P_1(0) = 1.0$. A plot of transition probability of particle in a box of length 2 box units as a function of time in optical cycle *i.e.* t/τ is shown in fig.1 for zero chirp, positive chirp and negative chirp rates. Here laser center frequency is set at $\omega_0 = 3/4$ *i.e.* resonant frequency between $n = 1$ and $n = 2$ state, the laser field strength *i.e.* E_0 is 1/8 and laser duration *i.e.* τ is 40.0.

Figure 1 shows that transition probability of $n = 2$ state is sufficiently large but there is some probability flow to higher states also and even there is probability flow to $n = 10$ state. At the end of the pulse the transition probabilities becomes constant. It is clear from figure that the variations in transition probabilities are compressed and stretched with the help of chirp. The transition probabilities show oscillatory behavior during the pulse. The higher states shows more oscillatory behavior as compared to $n = 1, 2$ or 3 state.

In **Figure 2** we have presented the variation of transition probability for different states as a function of laser chirp. The results here are taken at the end of the pulse. In this case central frequency ω_0 has been taken as 1/8 for *a, b* and 3/8 for *c, d*. Also laser duration τ is 40.0 for *a, d* and 80.0 for *b, c* subfigures. This is useful in com-
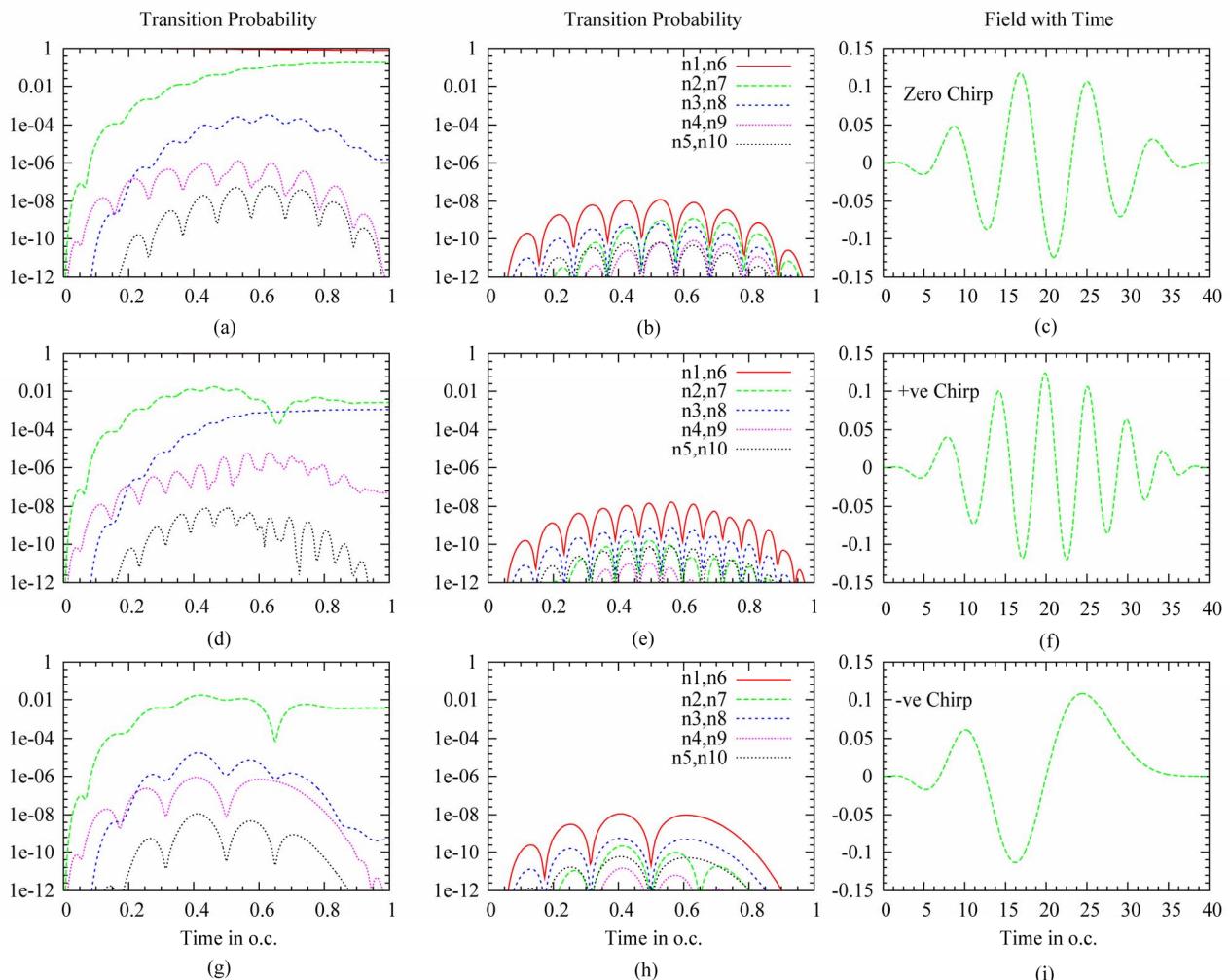

Figure 1. Transition probability of particle in a box in laser field as a function of time in optical cycle. Box width is 2×10^{-10} m. Laser center frequency is 3/4, laser duration $\tau = 40$ and field amplitude $E_0 = 1/8$. In Figure 1 (*a, b, c*) $\beta = 0.0$, Figure 1 (*d, e, f*) $\beta = + 1.0 \times 10^{-2}$ and Figure 1 (*g, h, i*) $\beta = -1.0 \times 10^{-2}$. Here, the key used explains that $n1$-$n5$ are for *a, d, g* and $n6$-$n10$ are for *b, e, h* subfigures. Subfigures *c, f, i* refers to the corresponding fields.
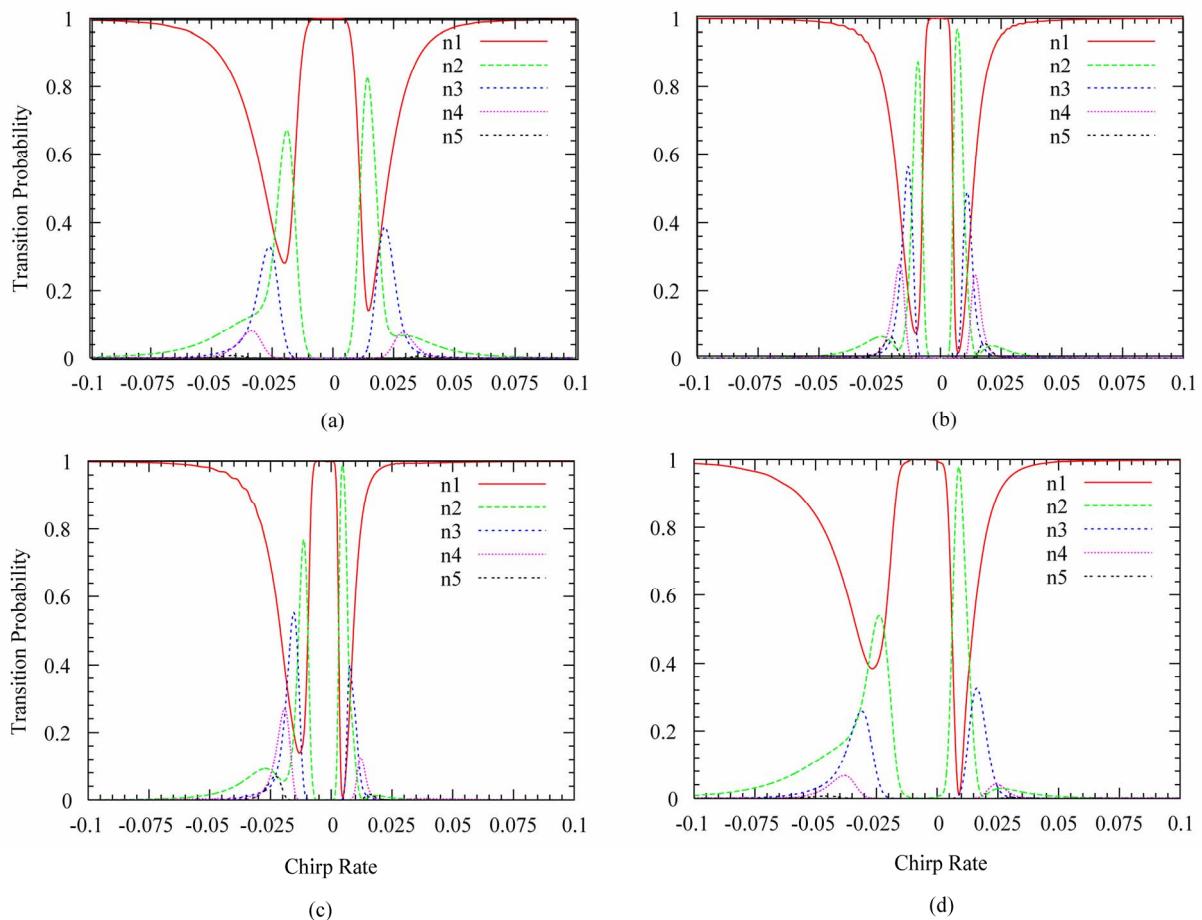
Figure 2. Transition probability for a particle in a box in chirped laser field as a function of chirp rate. Field strength E_0 = 1/2 and box length = 2.0. The centre frequency ω_0 = 1/8 for *a*, *b* and ω_0 = 3/8 for *c*, *d* subfigures. While the pulse width τ = 40.0 for *a*, *d* and τ = 80.0 for *b*, *c* subfigures. The results are taken at the end of the pulse.

paring the results for variation of transition probability of different states as a function of chirp rate (β) for two different frequencies and laser durations simultaneously. As it can be seen from figure that transition probabilities of $n = 3$ state is higher for negative chirp than positive chirp for $\tau = 40.0$ but it changes behviour for $\tau = 80.0$, although transition probability for n = 1 and n = 2 states increases as frequency ω_0 changes from 1/8 to 3/8 and transition probability remains greater for positive chirp than negative chirp. This change in probability shows that probability also depends on exposer time. Further, **Figure 2** also shows that almost complete population inversion can be achieved by chirped laser pulses. There is substantial population transfer to higher states also.

Figure 3 represents the transition probability of 5 states as a function of box length. The results are taken at the end of the pulse. It is clear from the figure that negatively chirped pulse connects higher states more effectively as compared to non-chirped pulse for the variation

in box length. Also (d) part shows that transition probability of different states changes drastically for the exposed time.

In **Figure 4**, we compare the transition probability for 5 states as a function of laser frequency. The results are taken at the end of the pulse. In part (b) the resonance between n = 1 and n = 2 states occurs at their natural frequency but in part (a) the chirp shifts the resonance and also it connects the higher order terms more efficiently.

6. Conclusions

The effect of chirped laser pulse on particle in a box has been studied and we have come to the conclusion that frequency modulated laser pulse is an effective approach to get system in excited state. The transition probability of different states as a function of different pulse parameters and the box length have been studied. The sys-
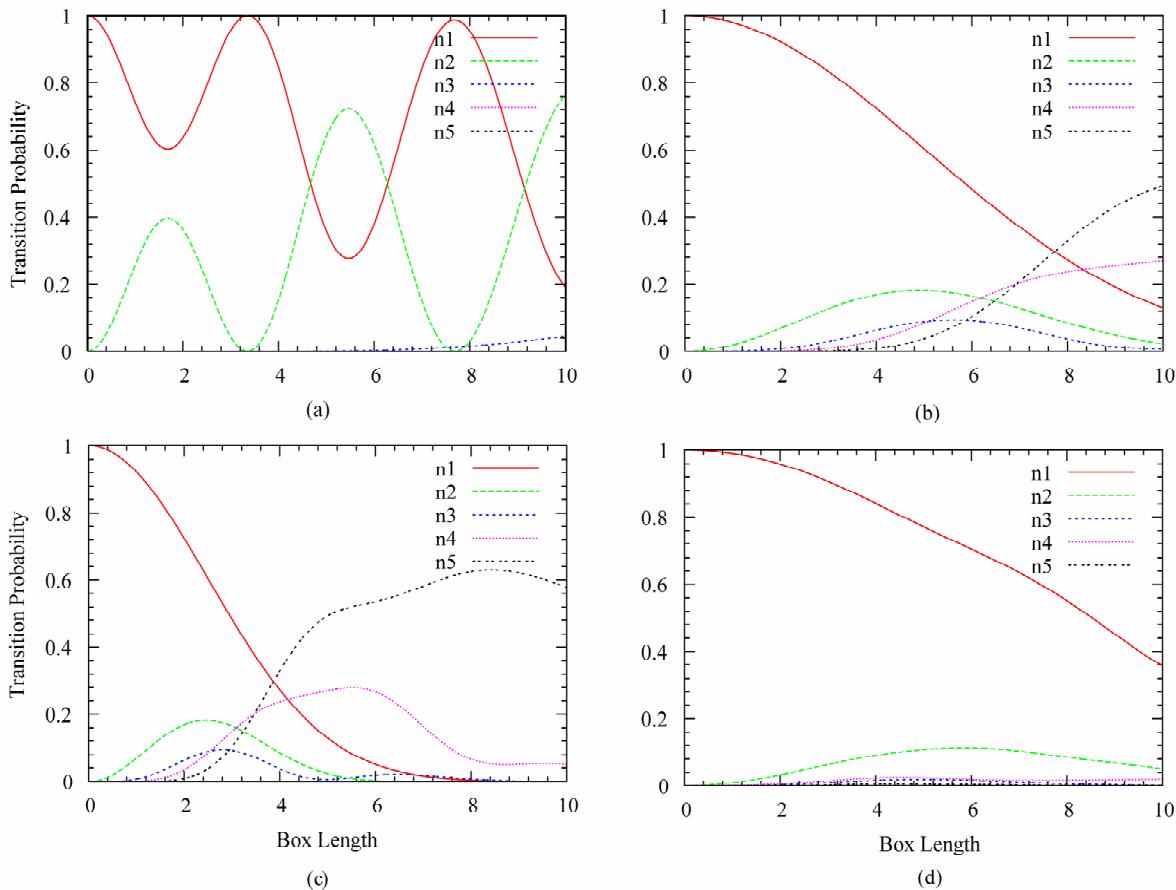
Figure 3. Transition probability of 5 states for particle in a box in chirped laser field as a function of box length. Chirp rate β = −5.0 × 10⁻² (except for (a) where β is zero), laser duration τ = 40 (except for (d) where τ is 80) and field amplitude E₀ = 1/2 (except for (b) where E₀ is 1/4).The results are taken at the end of the pulse.
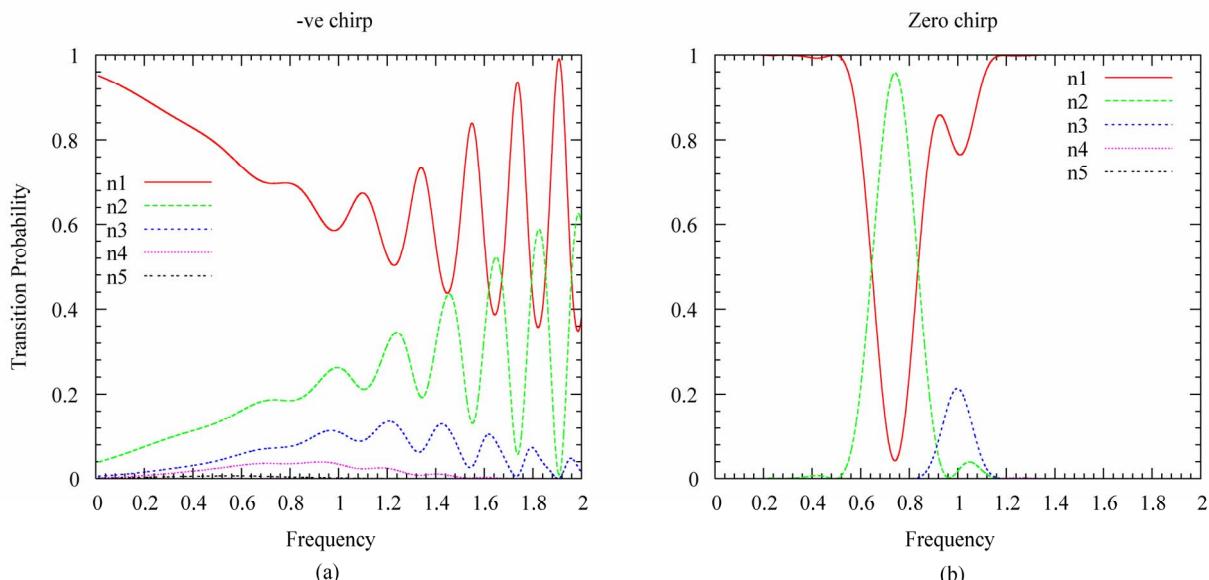

Figure 4. Transition probability of 5 states for particle in a box in chirped laser field as a function of central frequency. Chirp rate in part (a) is β = −5.0 × 10⁻² and zero in part (b). Laser duration is τ = 40, box length is 2.0 and field amplitude E₀ = 1/2.The results are taken at the end of the pulse.

tem is not merely two level shifting but with the help of chirped laser pulse we can shift the system to higher states, even n = 10 state has some transition probability (whatever small, it may be). The main result of the study is the variation in the dynamics due to time varying external potential and large transition probabilities for higher states in the presence of chirped laser pulse which can't be achieved with non-chirped pulse. The system remains in higher state for appreciable time that may help in many physical and chemical aspects.

7. Acknowledgements

8. References

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