Non linear response of a deformed oscillator

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Abstract

We analize the response of a single anharmonic diatomic molecule to a monochromatic time dependent electric field $\vec{E}_\omega(t)$ and evaluate the temporal evolution of the dipole moment, phase space trajectories and several transition probabilities as a function of the intensity of the field. We define deformed boson operators $A^\dagger = f(\hat{n})a^\dagger$, $A = af(\hat{n})$ in terms of the usual harmonic oscillator creation and annihilation operators a, $a^\dagger$, $\hat{n} = a^\dagger a$ and choose the number operator function $f(\hat{n})$ such that the energy spectrum of a harmonic oscillator-type Hamiltonian written in terms of the deformed operators yield an energy spectra similar to that of a Morse potential.

1 Theory

Much work has been devoted to the study of the optical linear and nonlinear response of harmonic systems to time dependent electric and magnetic fields either with classical [1] or quantum mechanical treatments [2, 3]. Laser pulses with well controlled temporal characteristics of amplitude and frequency have a high potential for selective manipulation of the internal state of atoms and molecules [4, 5, 6]. Cooling techniques have allowed the trapping and manipulation of atoms by optical means, however, fluctuations of the electromagnetic fields used to trap or to modify the quantum state lead to decoherence in ion traps and limits the trap stability[7]. A study involving multiple photon excitation for a linearly driven anharmonic oscillator using classical and quantum dynamics showed that the anharmonic nature of the Morse potential reduces de coherence of the quantum excitation process after the absorption of a few quanta[8]. In a recent work we analyzed the dipole moment nonlinearly induced by a space and time dependent field acting on a harmonic molecule; there, the origin of the nonlinearity is the quadrupolar coupling between the system and the field. The algebraic nature of the Hamiltonian is such that it was possible to obtain an exact solution to the problem in terms of functions which fulfill a set of nonlinear, coupled, first order differential equations which were solved numerically. For small field amplitudes our results conform with those of perturbation theory however, at high enough fields they differ significantly from the power law behavior predicted by perturbation theory. Whenever the driving frequency is close to a subharmonic of the resonance frequency, the high field signal is dominated by its n-th harmonic component [9].

In this work we generalize the algebraic method used in the harmonic case and apply it to an anharmonic system in order to study the effects due to the asymmetry of the potential and the consequences of having a finite number of bound states.

2 Algebraic Hamiltonian for the Morse Oscillator

A deformed oscillator is a non-harmonic system characterized by a Hamiltonian of the harmonic oscillator form,

$$H_D = \frac{\hbar\Omega}{2}\left(A^\dagger A + AA^\dagger\right), \tag{1}$$

with a specific frequency Ω and deformed boson *creation* and *anihilation* operators [10]

$$A = af(\hat{n}) = f(\hat{n}+1)a, \quad A^\dagger = f(\hat{n})a^\dagger = a^\dagger f(\hat{n}+1), \tag{2}$$

which differ from the corresponding harmonic operators $a^\dagger$ and a through an excitation level dependent deformation $f(\hat{n})$, where $\hat{n} = a^\dagger a$ is the harmonic number operator. The function f fixes the nonlinearity of the system. As $[a, a^\dagger] = 1$, the deformed operators obey the commutation relation

$$[A, A^\dagger] = (\hat{n}+1)f^2(\hat{n}+1) - \hat{n}f^2(\hat{n}). \tag{3}$$

Thus, the Hamiltonian may be written as

$$H_D = \frac{\hbar\Omega}{2}\left(\hat{n}f^2(\hat{n}) + (\hat{n}+1)f^2(\hat{n}+1)\right). \tag{4}$$

Notice that the eigenfunctions $|n\rangle$ of the harmonic oscillator are also eigenfunctions of the deformed oscillator. By choosing the deformation function $f(\hat{n})$ such that

$$f^2(\hat{n}) = 1 - \chi\hat{n}, \tag{5}$$

and choosing the anharmonicity parameter $\chi = 1/(2N+1)$ with integer N, the Hamiltonian becomes

$$H_D = \hbar\Omega\left(\hat{n} + 1/2 - \chi(\hat{n}+1/2)^2 - \chi/4\right), \tag{6}$$

whose spectrum differs only by a constant from the spectrum

$$E_M = \hbar\Omega\left(n + \frac{1}{2}\right) - \frac{\hbar\Omega}{2N+1}\left(n + \frac{1}{2}\right)^2 \tag{7}$$

of the Morse potential [11] with $N+1$ bound states corresponding to the integers $0 \leq n \leq N$. The Hamiltonian (6) contains an harmonic term plus a non linear contribution quadratic in the number operator, as well as an unimportant energy shift.

Substituting Eq. 5 into (2) we obtain the commutators

$$[A, A^\dagger] = 1 - (2\hat{n}+1)\chi, \quad [\hat{n}, A] = -A, \quad [\hat{n}, A^\dagger] = A^\dagger, \tag{8}$$

which approach the harmonic oscillator commutation relations as the number of bound states supported by the potential increases.

In the following we will employ Eq. (6) as an algebraic Hamiltonian that describes a Morse-like oscillator, provided we constrain the Hilbert space to that spanned by the $N+1$ states $|0\rangle \ldots |N\rangle$. As the Morse oscillator would be close to dissociation whenever $n \approx N$ and our algebraic Hamiltonian (6) has only discreet eigenstates, our approach is restricted to processes in which only low lying states $n \ll N$ participate.

3 Interaction with a driving field

We now analyze the response of the deformed oscillator to a time dependent potential. This kind of interaction is present in various physical situations, for instance, in a head on collision between an atom and a diatom, or when a molecule is driven by an oscillating classical electric field $E(t)$. We concentrate on the later case and study the response of a single polar molecule modeled by a Morse-like deformed oscillator dipolarly coupled to a time dependent field $E(t)$. To lowest order, the interaction potential is given by

$$V(t) = -qxE(t), \tag{9}$$

where q is the dynamic charge, and x is the relative coordinate measured from its equilibrium position. For simplicity, we have assumed that the system is one dimensional (x and E point in the same direction) and neglected the transverse nature of the electromagnetic field and any magnetic effects.

By identifying the number states $|n\rangle$ with the Morse eigenfunctions $\phi_n(x)$ and comparing the matrix elements [13] $\langle\phi_{n+\alpha}|x|\phi_n\rangle$ and $\langle\phi_{n+\alpha}|p|\phi_n\rangle$ of the position x and the momentum p operators with those of the deformed boson operators $\langle n+\alpha|(A^\dagger)^\alpha|n\rangle$ and $\langle n-\alpha|A^\alpha|n\rangle$ we may obtain expressions for x and p in terms of $\hat{n}$, A and $A^\dagger$,

$$x \simeq \sqrt{\frac{\hbar}{2m\Omega}}\left(f_{00} + f_{10}A^\dagger + Af_{01} + f_{20}(A^\dagger)^2 + A^2 f_{02} + \ldots\right), \tag{10}$$

$$p \simeq i\sqrt{\frac{\hbar m\Omega}{2}}\left(g_{10}A^\dagger + Ag_{01} + g_{20}(A^\dagger)^2 + A^2 g_{02} + \ldots\right), \tag{11}$$

where we only show terms with up to two boson excitations, i.e., of order A^2 and $(A^\dagger)^2$. The coefficients f_{ij}, g_{ij}, are functions of the excitation number operator $\hat{n}$ and are given by [13]

$$f_{00} = \sqrt{k}\left[f_0 + \ln\left(\frac{(k-2)(k-\hat{n}-1)}{(k-1-2\hat{n})(k-2\hat{n})}\right)(1-\delta_{\hat{n},0})\right], \tag{12}$$

$$f_{10} = f_{01} = \sqrt{\frac{k-1}{k}}\left(1 + \frac{\hat{n}}{k-\hat{n}}\right), \tag{13}$$

$$f_{20} = f_{02} = \frac{k-1}{2k\sqrt{k}}\left(\frac{-1}{(1-(\hat{n}-1)/k)(1-\hat{n}/k)}\right), \tag{14}$$

$$g_{10} = -g_{01} = \sqrt{\frac{k-1}{k}}\left(\frac{k-2\hat{n}}{k-\hat{n}}\right), \tag{15}$$

$$g_{20} = -g_{02} = -\frac{k-1}{k\sqrt{k}} \left(\frac{k-(2\hat{n}-1)}{k(1-(\hat{n}-1)/k)(1-\hat{n}/k)} \right), \tag{16}$$

and where

$$f_0 = \ln k - \left(\sum_{p=1}^{k-2} \frac{1}{p} - \gamma \right), \tag{17}$$

with

$$\gamma = \lim_{m\to\infty} \left(\sum_{p=1}^{m} \frac{1}{p} - \ln m \right) = 0.577216 \tag{18}$$

the Euler constant [14] and where $k = 2N+1 = 1/\chi$ is Child's parameter. The relative importance of one, two and more boson excitations in Eqs. (10) and (11) depend on the number of bound states N and on the excitation number n. For the parameters employed below, we have verified that the terms we keep are the dominant ones.

4 Response to a driving field

To simplify the presentation of our algebraic method, in a first approximation we calculate the response to a time dependent field by further simplifying Eq. (10), dropping the nonlinear two boson excitations, and keeping only constant and linear terms,

$$x = \sqrt{\frac{\hbar}{2m\Omega}} \left(f_{00} + f_{10} A^\dagger + A f_{10} \right), \tag{19}$$

$$p = i\sqrt{\frac{\hbar m\Omega}{2}} \left(g_{10} A^\dagger - A g_{10} \right), \tag{20}$$

In order to find the temporal evolution of the system, we write the time evolution operator in a product form $U(t) = U_0(t) U_I(t)$, where

$$U_0(t) = \exp\left(-\frac{i}{\hbar} H_D t \right). \tag{21}$$

is the unperturbed evolution generated by the deformed Hamiltonian (6) and the evolution operator in the interaction picture $U_I(t)$ obeys the differential equation

$$i\hbar \partial_t U_I(t) = (U_0(t)^\dagger V(t) U_0(t)) U_I(t) \equiv H_I(t) U_I(t), \tag{22}$$

with the initial condition $U_I(t_0) = 1$. The reference time t_0 is chosen so that the interaction is null or insignificant for previous times $t < t_0$.

To construct the operator $H_I(t)$ we must first transform the interaction (9) with the unperturbed evolution. To that end, we consider the transformations

$$\begin{aligned} A(t) &= U_0^\dagger(t) A U_0(t) = U_0^\dagger(t) a U_0(T) f(\hat{n}) \\ &= e^{-i\Omega t(1-2\chi(\hat{n}+1))} a f(\hat{n}) = e^{-i\Omega t(1-2\chi(\hat{n}+1))} A, \end{aligned} \tag{23}$$

$$\begin{aligned} A^\dagger(t) &= U_0^\dagger(t) A^\dagger U_0(t) = f(\hat{n}) U_0^\dagger(t) a^\dagger U_0(t) \\ &= f(\hat{n}) a^\dagger e^{i\Omega t(1-2\chi(\hat{n}+1))} = A^\dagger e^{i\Omega t(1-2\chi(\hat{n}+1))}. \end{aligned} \tag{24}$$

The interaction Hamiltonian is then

$$\begin{aligned} H_I &= -q\sqrt{\frac{\hbar}{2m\Omega}} \\ &\times \left(f_{00} + e^{-i\Omega t(1-2(\hat{n}+1)\chi)} A f_{10} + f_{10} A^\dagger e^{i\Omega t(1-2(\hat{n}+1)\chi)}\right) E(t). \end{aligned} \tag{25}$$

As the Hamiltonian contains the number operator in the exponential functions as well as in f_{00} and f_{10}, the set of operators appearing in H_I does not close under the operation of commutation. However, it would close if we replace the number operator $\hat{n}$ by some representative value $\tilde{n}$, leading to an *effective* frequency $\Omega_{\tilde{n}} = \Omega(1 - 2(\tilde{n}+1)\chi)$. The *constant number* $\tilde{n}$ will be defined later.

Within this approximation the interaction picture Hamiltonian becomes a simple linear combination of the operators $\{a, a^\dagger, 1\}$

$$\begin{aligned} H_I(t) &= -q\sqrt{\frac{\hbar}{2m\Omega}} \left(f_{00}(\tilde{n}) + f_{10}(\tilde{n}) f(\tilde{n}) (e^{-i\Omega_{\tilde{n}}(t-t_0)} a + a^\dagger e^{i\Omega_{\tilde{n}}(t-t_0)})\right) E(t) \\ &= \phi_0(t) + \phi_+(t) a^\dagger + \phi_-(t) a \end{aligned} \tag{26}$$

and consequently, the time evolution operator can be written *exactly* as a product of exponentials [15, 16]:

$$U_I = e^{-\beta_+ a^\dagger} e^{-\beta_- a} e^{-\beta_0} \tag{27}$$

with complex functions $\beta_i(t)$, $i = 0, +, -$ such that

$$\partial_t \beta_+ = \frac{i}{\hbar} \phi_+, \tag{28}$$

$$\partial_t\beta_- = \frac{i}{\hbar}\phi_-, \tag{29}$$

$$\partial_t\beta_0 = \frac{i}{\hbar}(\phi_0 - \phi_-\beta_+), \tag{30}$$

with initial conditions $\beta_i(t_0) = 0$, as required by $U_I(t_0) = 1$.

We can choose an adiabatically switched monochromatic electric field $E(t) = E_0\cos(\omega t)e^{\eta t}$ with a small switching rate η, in which case we can integrate analytically the differential equations and obtain

$$\begin{aligned}\beta_+ &= \sqrt{\frac{\hbar}{2m\Omega}}\frac{q}{2\hbar}f_{10}(\tilde{n}+1)f(\tilde{n}+1)e^{i\Omega_{\tilde{n}}(t-t_0)} \\ &\times\left(\frac{e^{i\omega t}}{\omega+\Omega_{\tilde{n}}-i\eta} - \frac{e^{-i\omega t}}{\omega-\Omega_{\tilde{n}}+i\eta}\right)E_0e^{\eta t},\end{aligned} \tag{31}$$

$$\begin{aligned}\beta_- &= \sqrt{\frac{\hbar}{2m\Omega}}\frac{q}{2\hbar}f_{10}(\tilde{n}+1)f(\tilde{n}+1)e^{-i\Omega_{\tilde{n}}(t-t_0)} \\ &\times\left(\frac{e^{i\omega t}}{\omega-\Omega_{\tilde{n}}-i\eta} - \frac{e^{-i\omega t}}{\omega+\Omega_{\tilde{n}}+i\eta}\right)E_0e^{\eta t}.\end{aligned} \tag{32}$$

Transforming the operators a and $a^\dagger$ with the time evolution operator in the interaction picture (see Eq. 27), we obtain:

$$U_I^\dagger a U_I = a - \beta_+ \tag{33}$$

$$U_I^\dagger a^\dagger U_I = a^\dagger + \beta_-. \tag{34}$$

From these, the coordinate operator x in the Heisenberg representation is:

$$x(t) = \sqrt{\frac{\hbar}{2m\Omega}}\left(f_{00} + f_{10}f_{\tilde{n}}\left(e^{-i\Omega_{\tilde{n}}t}(a-\beta_+) + (a^\dagger+\beta_-)e^{i\Omega_{\tilde{n}}t}\right)\right), \tag{35}$$

and the deformed dipole moment $q\langle n|x|n\rangle = \alpha E(t)$:

$$q\langle x(t)\rangle = q\sqrt{\frac{\hbar}{2m\Omega}}\left(f_{00} + f_{10}f_{\tilde{n}}\left[-e^{-i\Omega_{\tilde{n}}t}\beta_+ + e^{i\Omega_{\tilde{n}}t}\beta_-\right]\right), \tag{36}$$

substituting the expressions we got for the $\beta_\pm$, $f_{\tilde{n}}$ and taking the limit $\eta \to 0$ we obtain the linear polarizability (for the deformed oscillator)

$$\alpha(\omega > 0) = f_{10}^2 f_{\tilde{n}}^2\left((\frac{\Omega_{\tilde{n}}}{\Omega})\frac{q^2/m}{\Omega_{\tilde{n}}^2-\omega^2} + i\pi\frac{q^2}{m}\delta(\omega-\Omega_{\tilde{n}})\right) \tag{37}$$

showing that the replacement of the number operator by a constant value $\tilde{n}$, has as a consequence that the response of a deformed oscillator to an homogeneous field is similar to that of a harmonic oscillator with the difference that the resonance frequency depends upon the excitation state and the intensity of the response also depends upon the excitation state through the parameters $f_{\tilde{n}}$ and f_{10}. In the large N limit, the anharmonicity parameter $\chi \to 0$, $f_{\tilde{n}} \to 1$, $f_{10} \to 1$ and this expression reduces to that of the harmonic oscillator, however, for a non negligible value of the anharmonicity parameter or a large $\tilde{n}$ the correction term may be of importance.

Notice that we could have chosen a different temporal dependence for the electric field, the applicability of the method we have employed does not depend upon this choice.

Consider now the expansion of the coordinate (see Eq. 10) keeping up to second order terms in the operators A, $A^\dagger$. The interaction potential for an homogeneous field is given by Eq. 9 so that the Hamiltonian in the interaction picture can now be written in the form:

$$H_I(t) = \sum_{0 \le i+j \le 2} \phi_{ij} a^{\dagger^i} a^j \equiv \sum_{l=1}^{6} f_l X_l \tag{38}$$

where we have replaced the number operator by a number, and we have chosen the following order for the operators:

$$X_1 \equiv a^\dagger a, \quad X_2 \equiv a^{\dagger^2}, \quad X_3 \equiv a^\dagger, \quad X_4 \equiv a, \quad X_5 \equiv a^2, \quad X_6 \equiv 1.$$

The functions f_l are given by:

$$\begin{aligned}
f_1 &= 0 \\
f_2 &= -q f_{\tilde{n}}^2 \sqrt{\frac{\hbar}{2m\Omega}} f_{20} E(r_0, t) e^{2i\Omega_{\tilde{n}} t} \\
f_3 &= -q f_{\tilde{n}} f_{10} \sqrt{\frac{\hbar}{2m\Omega}} E(r_0, t) e^{i\Omega_{\tilde{n}} t} \\
f_4 &= -q f_{\tilde{n}} f_{10} \sqrt{\frac{\hbar}{2m\Omega}} E(r_0, t) e^{-i\Omega_{\tilde{n}} t} \\
f_5 &= -q f_{\tilde{n}}^2 \sqrt{\frac{\hbar}{2m\Omega}} f_{20} E(r_0, t) e^{-2i\Omega_{\tilde{n}} t} \\
f_6 &= -q \sqrt{\frac{\hbar}{2m\Omega}} f_{00} E(r_0, t)
\end{aligned}$$

notice that the coefficients responsible of processes of two quanta (f_2 and f_5) come from the second order terms in the expansion of the coordinate so that, even for a homogeneous field, the Morse potential gives rise to second harmonic generation.

The relative of importance of the different terms in the expansions for the coordinate and the momentum depend upon the excitation number $\tilde{n}$. For a fixed value of the Child parameter k, f_{10} and f_{20} vary slowly as functions of $\tilde{n}$ while f_{00} increases rapidly as $\tilde{n}$ approaches N; g_{10} and g_{20} are also slowly varying functions of $\tilde{n}$. For the numerical cases we have analyzed, corresponding to systems with $N = 15$, $N = 30$ and $N = 50$ the relations $|f_{00}| > |f_{01}| > |f_{02}|$ and $|g_{10}| > |g_{20}|$ are fulfilled. Thus we have disregarded higher than quadratic terms in f_{20}.

The set of operators appearing in H_I forms a finite Lie algebra so that the time evolution operator in the interaction picture can be written in a product form:

$$U_I(t) = e^{-\alpha_1(t)a^\dagger a} e^{-\alpha_2(t)a^{\dagger 2}} e^{-\alpha_3(t)a^\dagger} e^{-\alpha_4(t)a} e^{-\alpha_5(t)a^2} e^{-\alpha_6(t)} \tag{39}$$

with the time dependent, complex functions α_n fulfilling a set of coupled, first order, nonlinear, differential equations which is obtained after substitution of Eq 39 into Eq. 22 [9]. These equations are solved numerically and the temporal evolution of any operator can then be calculated. In particular, the temporal evolution of the coordinate is given by:

$$x(t) = \sqrt{\frac{\hbar}{2m\Omega}} U_I^\dagger U_0^\dagger \left(f_{00} + f_{10} A^\dagger + A f_{01} + f_{20} (A^\dagger)^2 + A^2 f_{02} \right) U_0 U_I \tag{40}$$

applying the transformations

$$\begin{aligned} U_I^\dagger U_0^\dagger A U_0 U_I &= f_{\tilde{n}} e^{-i\Omega_{\tilde{n}} t} e^{-\alpha_1} (a(1 - 4\alpha_2\alpha_5) - 2\alpha_2 a^\dagger - (\alpha_3 + 2\alpha_2\alpha_4)) \\ &\equiv t_1 a + t_2 a^\dagger + t_3 \qquad (41) \\ U_I^\dagger U_0^\dagger A^\dagger U_I U_0 &= f_{\tilde{n}} e^{i\Omega_{\tilde{n}} t} e^{\alpha_1} (2\alpha_5 a + a^\dagger + \alpha_4) \\ &\equiv t_4 a + t_5 a^\dagger + t_6. \qquad (42) \end{aligned}$$

and taking the average value between number eigenstates we get:

$$\begin{aligned} \langle n | x(t) | n \rangle &= \sqrt{\frac{\hbar}{2m\Omega}} (f_{00} + f_{10}(t_3 + t_6) \\ &+ 2 f_{20}((t_1 t_2 + t_4 t_5) n + (t_1 t_2 + t_4 t_5 + t_3^2 + t_6^2))). \qquad (43) \end{aligned}$$

5 Transition probabilities

Once we have the explicit form for the time evolution operator, we can evaluate the transition probability from an initial state n to a final state n' of the oscillator

$$P_{n,n'}(t) = |A_{n,n'}(t)|^2 = |\langle n'|U_I(t)|n\rangle|^2. \tag{44}$$

To do that, we substitute the explicit form of the time evolution operator $U_I(t)$ (see Eq. 39)

$$A_{n,n'} = e^{-\alpha_6} e^{-\alpha_1 n'} \langle n'| e^{-\alpha_2 a^{\dagger 2}} e^{-\alpha_3 a^\dagger} e^{-\alpha_4 a} e^{-\alpha_5 a^2} |n\rangle. \tag{45}$$

Expanding the exponentials $e^{-\alpha_4 a} e^{-\alpha_5 a^2}$ and acting upon the state $|n\rangle$, we get two finite summations

$$\begin{aligned} e^{-\alpha_4 a} e^{-\alpha_5 a^2} |n\rangle &= e^{-\alpha_4 a} \sum_{k=0}^{[\frac{n}{2}]} \frac{(-\alpha_5)^k}{k!} \sqrt{\frac{n!}{(n-2k)!}} |n-2k\rangle \\ &= \sum_{k=0}^{[\frac{n}{2}]} \frac{(-\alpha_5)^k}{k!} \sum_{l=0}^{n-2k} \frac{(-\alpha_4)^l}{l!} \sqrt{\frac{n!}{(n-2k-l)!}} |n-2k-l\rangle. \end{aligned}$$

The other two exponentials are expanded and applyed to the final state $\langle n'|$

$$\langle n'| e^{-\alpha_2 a^{\dagger 2}} e^{-\alpha_3 a^\dagger} = \sum_{p=0}^{[\frac{n'}{2}]} \frac{(-\alpha_2)^p}{p!} \sum_{q=0}^{n'-2p} \frac{(-\alpha_3)^q}{q!} \sqrt{\frac{n'!}{(n'-2p-q)!}} \langle n'-2p-q|$$

so that, the final expression for the probability amplitude $A_{n,n'}$ is:

$$\begin{aligned} A_{n,n'} = \; & e^{-\alpha_6 - \alpha_1 n'} \sum_{k=0}^{[\frac{n}{2}]} \frac{(-\alpha_5)^k}{k!} \sqrt{\frac{n!}{(n-2k)!}} \sum_{l=0}^{n-2k} \frac{(-\alpha_4)^l}{l!} \sum_{p=0}^{[\frac{n'}{2}]} \frac{(-\alpha_2)^p}{p!} \\ & \times \sum_{q=0}^{n'-2p} \frac{(-\alpha_3)^q}{q!} \delta_{n-2k-l,n'-2p-q} \end{aligned} \tag{46}$$

with all the summations finite.

6 Numerical results

For the numerical evaluation of the response we choose systems with anharmonicity parameters $\chi = 0.032$, $\chi = .016$ and $\chi = .0099$ corresponding to $N = 15$, $N = 30$ and $N = 50$ respectively and set the constant number $\tilde{n}$ as the initial state of the system. To produce Fig. 1 we choose a small switching rate $\eta = 0.0002$ and an initial time $|t_0| \gg 1/\eta$ such that $e^{\eta t_0} < 10^{-5}$.

In Fig. 1 we show the last 10 periods of the temporal evolution of the dipole moment as a function of time for $N = 15$ with a homogeneous field and $E_0 = .25\mathcal{E}$, where $\mathcal{E}=\hbar\Omega/q\ell$ is the field that would produce an appreciable energy change, of the order of the vibration energy quantum when a charge q is displaced a distance of the order of a typical vibration amplitude $\ell = \sqrt{\hbar/m\Omega}$. We set $\omega = .24\Omega$, so that nonlinear processes corresponding to the fourth harmonic are resonant. Using the linear expression (see Eq.37) the system responds with the forcing frequency ω and the amplitude of the oscillations is symmetric with respect to the origin (full line). Using the numerical solution given by Eq. 43 where non linear terms in the expansion of the coordinate have been kept, we see that the deformed system also responds with the forcing frequency but the amplitude of the vibrations is not symmetrical with respect to the origin due to the asymmetry of the Morse potential.

In figure 2 we show one period of the phase space trajectory $\langle x \rangle$ *vs* $\langle p \rangle$ for the deformed oscillator with $N = 15$, $n_i = 0$ and several values for the intensity of the field. The innermost trajectory corresponds to a small intensity $E_0 = .25\mathcal{E}$, here the trajectory resembles that of a harmonic oscillator, the next one corresponds to $E_0 = .5\mathcal{E}$ and the non linear terms begin to play a role, the trajectory is no longer a ellipse but it acquires a slight deformation, finally for $E_0 = .75\mathcal{E}$ the deformation is much more significant.

In figure 3 we show the last period of the phase space trajectory $\langle x \rangle$ *vs* $\langle p \rangle$ for a deformed oscillator with $N = 15$ (full line), $N = 30$ (broken line) and $N = 50$ (dashes) for a homogeneous field with $\eta = 0.0002$, $E_0 = .75\mathcal{E}$ and a forcing frequency $\omega = .34\Omega_0$. Though the average phase space trajectory reminds us of that of a harmonic oscillator, in particular the one with $N = 50$ which approaches an ellipse, it is clear that for this value of the intensity of the field the non linear effects are evident since the trajectory for the other two cases is not an ellipse, indicating the presence of more than one frequency in the system's response. As is to be expected, the relevance of the nonlinearities increases with the anharmonicity parameter.

In order to study the transition probabilities, we considered a pulsed electric field of the form $E(t) = E_0 e^{-\eta t^2} \cos\omega t$ with $\eta = 0.001$ and the initial time for integration such that $e^{-\eta t_0^2} < 10^{-5}$. In figure 4 we show twenty periods (from -10τ to 10τ, $\tau = 2\pi/\omega$) of the temporal evolution of the transitions

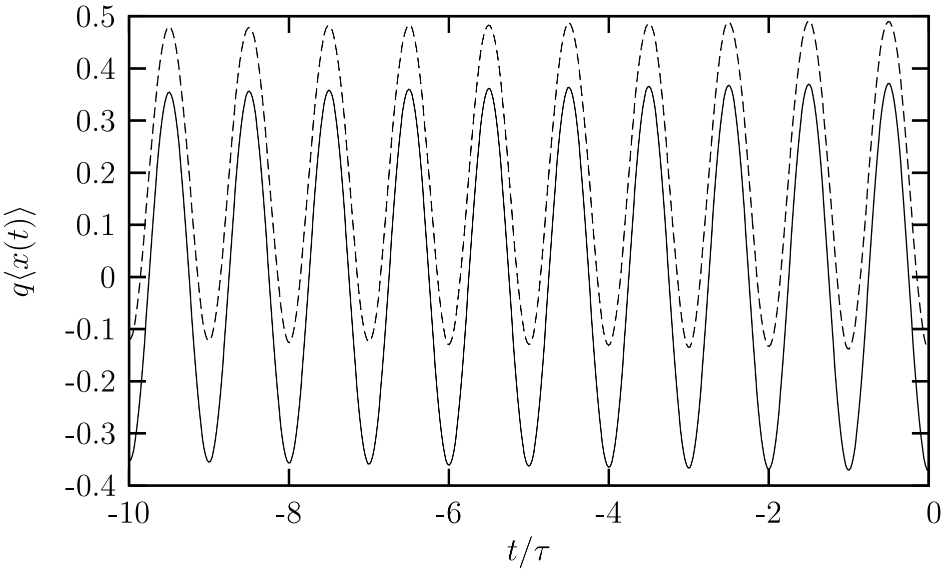

Figure 1: Dipole moment $q\langle x(t)\rangle$ as a function of time in units of the period $\tau = 2\pi/\omega$ for an anharmonic molecule in the presence of a homogeneous field in the linear (full line) and numerical (dashes) approaches discused in the text. The parameters used are: $\eta = 0.0002$, $N = 15$, $\omega = 0.24\,\Omega_0$ and $E_0 = .3\mathcal{E}$.

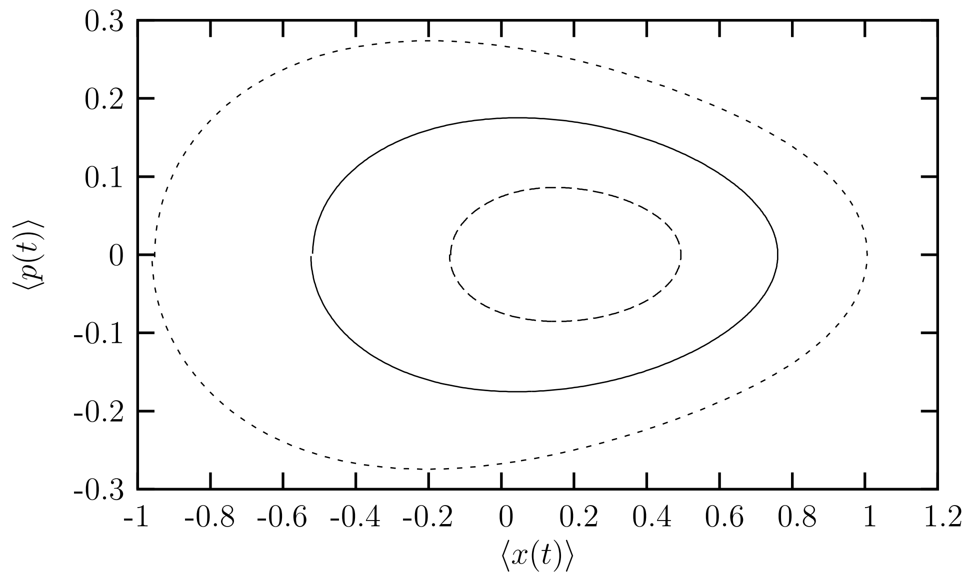

Figure 2: Phase space trajectory $\langle x(t)\rangle$ *vs* $\langle p(t)\rangle$ for a field with frequency $\omega = .24\Omega_0$, swtching rate parameter $\eta = 0.0002$ and amplitudes $E_0 = .25\mathcal{E}$(broken line), $E_0 = .5\mathcal{E}$ (full line) and $E_0 = .75\mathcal{E}$ (dashes) acting on a deformed oscillator with $N = 15$, $n_i = 0$.

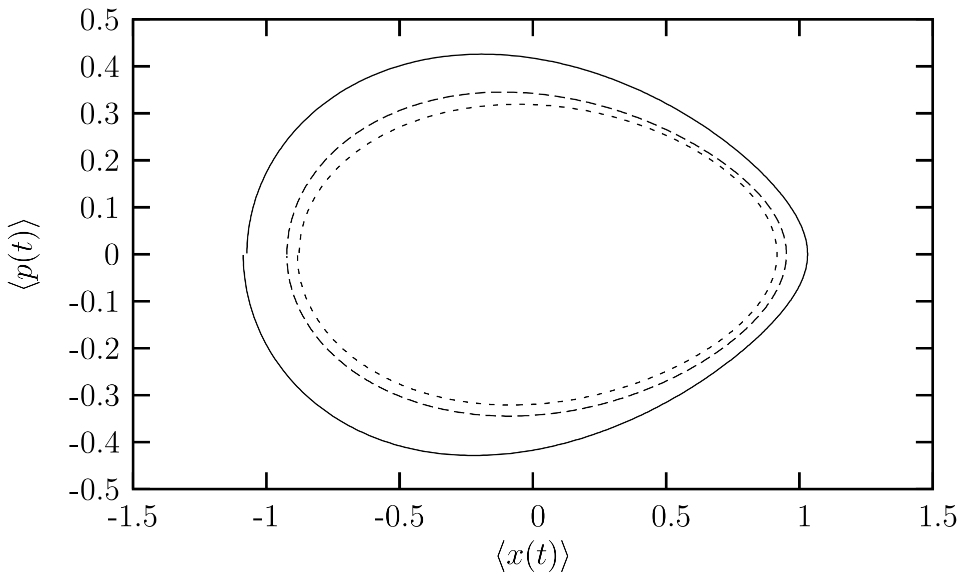

Figure 3: Last period of the phase space trajectory $\langle x(t)\rangle$ *vs* $\langle p(t)\rangle$ for a forcing field with $E_0 = .75\mathcal{E}$, $\omega = .34\Omega_0$, $\eta = 0.0002$ and deformed oscillators with $n_i = 0$ and $N = 50$ (dashes), $N = 30$ (broken line) and $N = 15$ (full line).

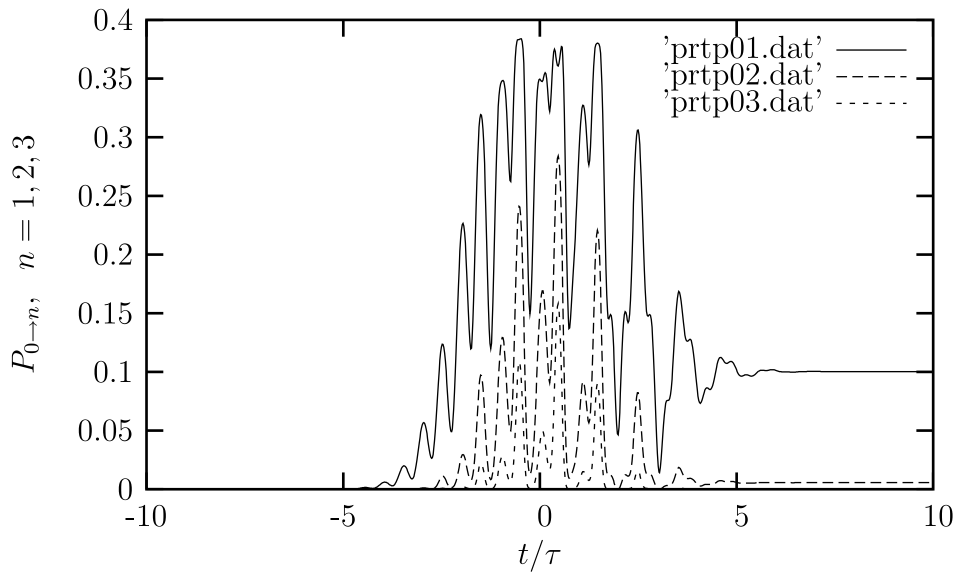

Figure 4: Transition probabilities (0-n) $n = 1, 2, 3$ as a function of time for $N = 30$, $E_0 = \mathcal{E}$, $\omega = .49\Omega$.

(0-1,0-2 and 0-3) for a deformed oscillator with $N = 30$, and a field with amplitude $E_0 = \mathcal{E}$ and frequency $\omega = .49\Omega$.

As the pulse impinges upon the system, at about -4τ the transition from the ground to the first excited state starts to build up oscillating with the field's frequency, later, at about -2τ the transition to the second excited state begins to be noticeable and a little later that to the third excited state. At all times, the (0-1) transition probability is larger than any other. Near $t = 0$ when the pulse is at its peak, the transition (0-1) shows oscillations with a larger frequency which indicates the effect of non linear terms in the interaction. As the pulse abandons the interacting region, the oscillations stop and the system arrives to a stationary state which is a combination of the ground state and the first excited state with a small contribution from higher states.

Finally, in Figs.5 and 6 we show the temporal evolution of the average value of the displacement $\langle x(t)\rangle$ and the phase space $\langle x(t)\rangle$ *vs* $\langle p(t)\rangle$ the for a deformed oscillator with $N = 30$ in an initial state $n_i = 0$ forced by a pulsed field characterized by an amplitude $E_0 = .75\mathcal{E}$, frequency $\omega = .34\Omega_0$, and

$\eta = 0.001$.

At the initial time when the oscillator is in the ground state, the average value of the coordinate is a constant displaced from the origin due to the function f_{00}. As the pulse arrives, the system starts to oscillate around this value with the field's frequency, as the interaction takes place, the system absorbs energy from the field, the amplitude of the oscillations increases and after the pulse is gone, the system arrives to an excited state evidenced by the small oscillations with a larger frequency than that of the forcing field.

Figure 6 shows the temporal evolution of the the phase space trajectory, we see that as the pulse arrives and the system starts to absorb energy, the average values of coordinate and momentum increase and the presence of nonlinear effects can be discerned since the trajectories are not ellipses, after the pulse is gone the average values of the momentum and the displacement oscillate around the initial value with a small amplitude showing that the system has arrived to an excited state.

7 Conclusions

The use of deformed oscillators with a deformation function adequate to reproduce the energy spectrum of a Morse potential [17], has lead us to a model for an anharmonic potential which supports a finite number of bound states. By choosing a slightly different form for $f(\hat{n})$, we could build an alternative Hamiltonian with a spectrum corresponding to the Pöschl-Teller Hamiltonian. The energy spectra of the deformed oscillator given by Eq. 6 has the same form as that of the Morse and the Pöschl-Teller potentials [11], however as a function of the displacement coordinate these potentials are very different. When one considers the expansion of the displacement coordinate in terms of the deformed operators, for the Pöschl-Teller case the expansion contains only odd powers of the creation and annihilation operators [12] while for the Morse case even and odd terms are present [13].

We saw that the linear response has similar forms in the harmonic and anharmonic cases with the difference that in the latter the resonance frequency of the oscillator depends upon the excitation state. We have shown that the non linear effects in the response of the anharmonic system increase with the amplitude of the field and when the field's frequency approaches the resonance frequency of the oscillator. Since our method can be applied to any temporal dependence, we analyzed the phase space trajectories for dif-

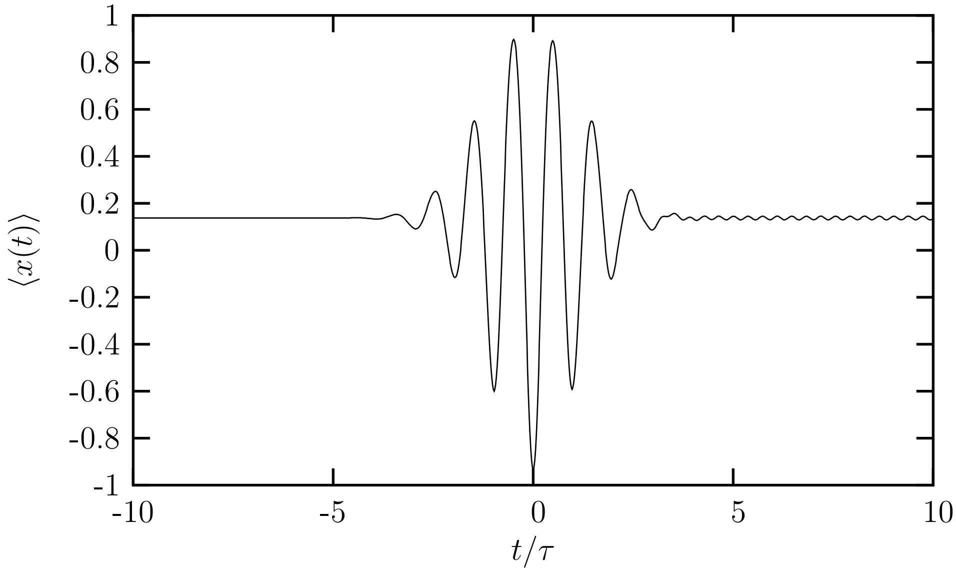

Figure 5: Temporal evolution of the displacement for a deformed oscillator with $N = 30$ initially in the ground state $n_i = 0$ subjected to a pulse with $E_0 = .75\mathcal{E}$, frequency $\omega = .34\Omega_0$ and $\eta = 0.001$

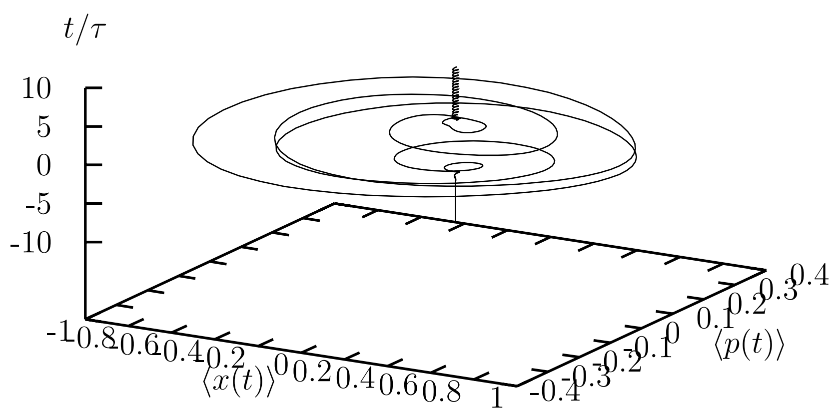

Figure 6: Temporal evolution of the phase space trajectories for a deformed oscillator with $N = 30$, in the ground state subjected to a pulsed field with $E_0 = .75\mathcal{E}$, $\omega = .34\Omega_0$, and $\eta = 0.001$

ferent temporal dependences of the field. When the number of bound states supported by the potential is large, the phase space trajectories resemble those of harmonic oscillators; for larger anharmonicity parameters (smaller number of bound states) they are no longer ellipses showing an indication of the relevance of the non linear effects.

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