Revista Colombiana de Física,Vol. 41, No.2, Abril 2009

Perturbed Hooke's Atom Exposed to Intense Ultrashort Laser Pulses

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Recibido 23 de Oct. 2007; Aceptado 6 de Mar. 2009; Publicado en línea 30 de Abr. 2009

Resumen

Se propone un método basado en la aproximación adiabática para estudiar la dinámica del átomo de Hooke cuántico con frecuencia armónica variable en interacción con pulsos láser intensos. Se demuestra que modificando este potencial de confinamiento en el tiempo, se puede enriquecer la dinámica de este sistema modelo, dado que, en ausencia de tal perturbación, sólo es posible encontrar dos regímenes posibles; transparencia total a la radiación, o bien, absorción total.

***Palabras Clave*:** Átomo de Hooke, Pulsos láser.

Abstract

We propose a method based on the adiabatic approximation to study the dynamics of the quantum Hooke's atom with varying oscillator frequency $\omega(t)$ when exposed to intense laser pulses. It is shown that by modifying this confinement potential in time, we may enrich the outcome of this model system given that, in absence of such perturbation, only total photo-transparency or total photo-absorption are possible.

***Keywords*:** Hooke's Atom, Laser pulses.

1. Introducción

The two-electron Hooke's atom is a model system similar to the Helium atom, where only the culombian potential due to the electron-nucleus interaction is replaced by that of an harmonic oscillator. This quantum system is known to have an analytical solution for a given set of oscillator frequencies [1]. Probably it is less known that the Hooke's atom subject to a radiation field is also one of those few time-dependent exactly solvable problems in Quantum Mechanics [2]. The underlying reason for the exact solution comes from the separability of the two-electron system in uncoupled center of mass and relative motions. Only the center of mass motion is affected by the radiation field and its associated equation is equivalent to that of the well-known forced harmonic oscillator (FHO). The latter system in one dimension has been analyzed in extension by Nogami [3] and Akridge [4], although to our surprise the solution is already outlined in a textbook back in the early 60's [5]. Curiously, the solution for the FHO merges the quantum motion with the classical one, in such a way that the wavepacket is driven by the classical trajectory. The relevant quantities to be calculated are transition probabilities between any two states and an analytical expression is readily available.

These ideas have been then extended to the full two-electron Hooke's atom [6]. The expression for the transition probabilities allows one to conclude that only two possible regimes are possible: first, when the radiation frequency ω_L is equal to the harmonic frequency ω (resonant case) the system absorbs every photon contained

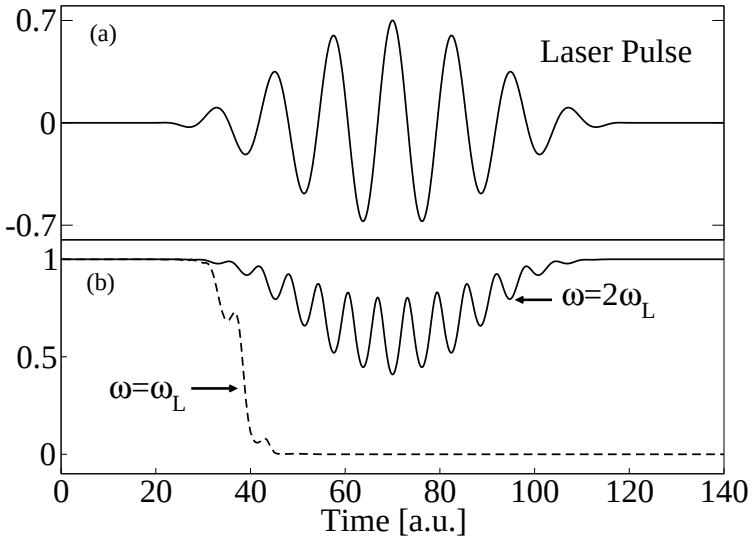

Figura 1. From top to the bottom: (a). Electric field $\mathbf{E}(t)$ of the laser pulse with parameters $\omega_L = 0{,}5$, $E_0 = 0{,}7$ and $T = 100$. (b) Time evolution of the ground state population $P_o(t)$ for the resonant case ($\omega = \omega_L$) with full depletion and the off-resonant case ($\omega = 2\omega_L$) with transparency.

in the pulse and the initial state becomes fully depleted, and second, if both frequencies are off resonance, the Hooke's atom never absorbs a net number of photons, i.e., its behaviour is transparency to the radiation. This characteristic dichotomy between full depletion or full transparency strongly reduces the possibility of controlling the system by tunable lasers. Therefore, in order to enrich the outcome of the Hooke's atom exposed to laser pulses, we propose also to vary the confinement frequency ω in time. An exact solution to this new problem is yet unknown. Then we must resort to the numerical solution of the time dependent Schrödinger equation (TDSE). A procedure to solve the TDSE with an adiabatic basis expansion is here proposed. Atomic units are used throughout unless otherwise stated.

2. Method of Solution

The TDSE for the Hooke's atom of varying frequency $\omega(t)$ subject to a radiation field $\mathbf{E}(t)$ in the dipolar approximation (length gauge) reads:

$$i\partial_t \Psi(\mathbf{r}_1,\mathbf{r}_2,t) = \Bigg[-\frac{1}{2}(\nabla_1^2+\nabla_2^2) + \frac{\omega^2(t)}{2}(r_1^2+r_2^2) + \frac{1}{r_{12}} - (\mathbf{r_1}+\mathbf{r_2})\cdot\mathbf{E}(t)\Bigg]\Psi(\mathbf{r}_1,\mathbf{r}_2,t) \tag{1}$$

For the laser pulse to be finite we use a cosine wave confined within a sine-squared envelope $\mathbf{E}(t) = E_0 \sin^2(\pi t/T)\cos[\omega_L(t-T/2)]\boldsymbol{\varepsilon}$, where E_0 is the peak amplitude for the electric field, T is the pulse duration and ω_L is the laser frequency. We also propose a periodic variation for the confinement, such that $\omega(t)$ is given by $\omega(t) = \omega_0 + (\omega_1 - \omega_0)\left(\sin[\pi(t/t_1 - 1/2)] + 1\right)/2$, where ω_0 and ω_1 are minimum and maximum values for ω, respectively and t_1 corresponds to the half period.

Using the new coordinates $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ Eq. (1) uncouples into

$$\left(i\partial_t + \frac{\nabla_R^2}{4} - \omega^2(t)R^2 + 2\mathbf{R}\cdot\mathbf{E}(t)\right)\Phi(\mathbf{R},t) = \left(i\partial_t + \nabla_r^2 - \frac{\omega^2(t)}{4}r^2 - \frac{1}{r}\right)\varphi(\mathbf{r},t) = 0 \tag{2}$$

where $\Phi(\mathbf{R},t)$ is the center of mass (CM) wavefunction and $\varphi(\mathbf{r},t)$ the wavefunction for the relative motion (RM), being the total function $\Psi(\mathbf{R},\mathbf{r},t) = \Phi(\mathbf{R},t)\cdot\varphi(\mathbf{r},t)$. These two TDSE equations admit an unifying compact notation:

$$\left(i\partial_t - \mathcal{H}_0^{\mathbf{Q}} - \mathcal{W}^{\mathbf{Q}}\right)\Upsilon(\mathbf{Q},t) = 0 \tag{3}$$

where $\mathbf{Q} = \{\mathbf{R},\mathbf{r}\}$, $\mathcal{H}_0^{\mathbf{R}} = -\frac{\nabla_R^2}{4} + \omega^2(t)R^2$, $\mathcal{H}_0^{\mathbf{r}} = -\nabla_r^2 + \frac{\omega^2(t)}{4}r^2 + \frac{1}{r}$, $\mathcal{W}^{\mathbf{R}} = -2\mathbf{R}\cdot\mathbf{E}(t)$ and $\mathcal{W}^{\mathbf{r}} = 0$. To solve Eq. (3) we make use of an adiabatic expansion in

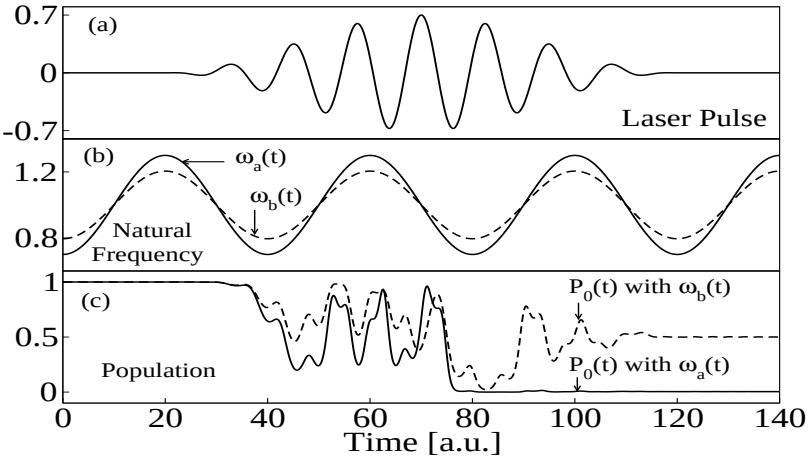

Figura 2. From top to the bottom: (a). Electric field $\mathbf{E}(t)$ of the laser pulse with parameters $\omega_L = 0{,}5$, $E_0 = 0{,}7$ and $T = 100$. (b) Variation of $\omega(t)$ with two sets of parameters $\omega_a = [\omega_0,\omega_1] = [0{,}70, 1{,}30]$ and $\omega_b = [0{,}795, 1{,}205]$ but the same $t_1 = 20$ (see text). (c) Time evolution of initial ground state population $P_0(t)$ for the two sets in (b).

terms of the instantaneous eigensolutions of $\mathcal{H}_0^{\mathbf{Q}}(\omega(t))$ (i.e., for every given ω at time t)

$$\Upsilon(\mathbf{Q},t) = \sum_n c_n^{\mathbf{Q}}(t)\cdot\psi_n(\mathbf{Q},\omega(t))\exp\left(-i\int_0^t E_n^{\mathbf{Q}}(\tau)d\tau\right) \tag{4}$$

This is an appropriate method when the perturbation varies smoothly. By inserting this ansatz into Eq. (3) one obtains a set of coupled equations:

$$\dot{c}_m^{\mathbf{Q}}(t) = \sum_n c_n^{\mathbf{Q}}(t)\left[-i\langle\psi_m|\partial_t|\psi_n\rangle + \langle\psi_m|\mathcal{W}^{\mathbf{Q}}(t)|\psi_n\rangle\right] \tag{5}$$

where the so called dynamical couplings $\langle\psi_m|\partial_t|\psi_n\rangle$ may be readily obtained using the Hellman-Feynman theorem, resulting into:

$$\begin{aligned}&\langle\psi_m(\mathbf{Q},\omega(t))|\partial_t|\psi_n(\mathbf{Q},\omega(t))\rangle = \\ &\beta^{\mathbf{Q}}\omega(t)\dot{\omega}(t)\langle\psi_m|Q^2|\psi_n\rangle/(E_n^{\mathbf{Q}}(t) - E_m^{\mathbf{Q}}(t))\end{aligned} \tag{6}$$

where $\beta^{\mathbf{R}} = 2$ and $\beta^{\mathbf{r}} = 1/2$. Dynamical couplings have a closed form for the CM motion. As mentioned above, the RM motion admits an exact solution for a discrete set of natural frequencies ω but we do require a solution for any arbitrary value of $\omega(t)$. We choose to expand the eigensolutions of $\mathcal{H}_0^{\mathbf{r}}$ in terms of B-splines basis sets, i.e., $\psi_n(\mathbf{r}) = \sum_i b_{ni}\cdot B_i^k(r)/r\cdot Y_{\ell m}(\theta,\phi)$, that provides a very accurate solution for the energies $E_n^{\mathbf{r}}$ and the couplings $\langle\psi_m|r^2|\psi_n\rangle$. At variance, dipolar matrix elements $\langle\psi_m(\mathbf{R},\omega(t))|\mathcal{W}^{\mathbf{R}}(t)|\psi_n(\mathbf{R},\omega(t))\rangle$, only relevant for the CM motion, are analytical. Since the variation of $\omega(t)$ is periodic in time, energies and couplings may be computed only once for a finite set of values in $[\omega_0,\omega_1]$, i.e., a set of instantaneous solutions is prepared in advance. Being so, we make use of an interpolation scheme for energies and couplings during the time propagation. This procedure turns out to be very accurate and stable when energies and couplings are continuous and vary smoothly. A Bulirsch-Stoer integrator has been used to propagate the set of coupled equations, subject to an initial condition where the Hooke's atom is in its ground state.

3.Results and Conclusions.

As mentioned in the Introduction, an exact solution for the Hooke's atom exposed to a radiation field may be obtained when the natural frequency ω is constant. From this solutions one may conclude that the Hooke's atom shows quite a particular behaviour in photoabsorption processes. A net photon (energy) absorption is only possible when the laser field is in resonance with the natural frequency ($\omega_L = \omega$). As a result the initial state becomes fully depopulated at the end of the pulse (see 1 *b*). For any other case being off resonance (including multiphoton transitions in the form $\omega = n\omega_L$) there is no photoabsorption after the field interaction, at variance with many other real atomic systems. Being off resonance, all the energy absorbed by the system is promptly released in a symmetrical reversible process. This effect of transparency is also illustrated in Figure 1 *b*.

A route to break down such simple behaviour in the Hooke's atom (either total depletion of the initial state or total transparency) is here proposed by using tunable natural frequencies $\omega(t)$. The picture at hand may be two electrons confined in an external time dependent harmonic potential and driven by a laser pulse. As

shown in Figure 2, by only varying the confinement with $\omega(t)$ is not enough to produce any meaningful effect on the initial state (please notice that the laser pulse starts at 20 a.u.). The dynamics with laser field and fixed $\omega(t) = 1 \ \forall \ t$ was included in Figure 1 b and shows transparency. It is just the joint effect of varying $\omega(t)$ and the laser pulse that produces a distinct behaviour, which is more amenable for dymanical control purposes. In Figure 2 we also illustrate how to manipulate the final outcome of the initial state population P_o by tuning $\omega(t)$ in a laser field. By changing the boundaries $[\omega_0,\omega_1]$ of $\omega(t)$ (see Figure 2 b), we may control the system to yield total absorption (even being off resonance since $\omega(t) \neq \omega_L \ \forall \ t$) or to select the final population of the initial state (in fact, for any state) at will (in Figure 2 c, if $P_0(T) = 0$ and $0{,}5$ are required, then $\omega(t)$ is shaped accordingly). The ideas here developed may find applications in the dynamics of particles confined by experimental Paul traps and exposed to intense laser fields.

Referencias

[1] M. Taut, *Phys. Rev. A*, **48**, 3561 (1993).
[2] U. Schwengelbeck, *Phys. Lett. A*, **253**, 168 (1999).
[3] Y. Nogami, *Am. J. Phys.*, **59**(1), 64 (1991)
[4] R. Akridge, *Am. J. Phys.*, **63**(2), 141 (1995)
[5] I.I. Gol'dman and V.D. Krivchenkov *Problems in Quantum Mechanics*, Pergamon Press (1961)
[6] O. Kidun and D. Bauer, *J. Phys. B*, **40**, 779 (2007).