DYNAMICS OF COUPLED ELECTRON - NUCLEON MOTION IN A LASER FIELD

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ABSTRACT

Energy transfer processes in single particle coupled nucleon-electron models interacting with an intense laser field are studied using semi-classical quantization of the coupled classical Hamiltonian.

INTRODUCTION

With the development of intense laser sources operating at higher powers, shorter pulse widths or shorter wavelengths, the study of intense laser-matter interactions is a growing area of science -- some current work centers around the use of laser produced plasmas as x-ray or x-ray laser sources. In addition, new and interesting areas are the study of above threshold ionization, ultraviolet multiphoton picosecond processes, multiphoton ionization and the production of harmonic radiations from atoms subjected to strong laser fields. In these areas of research the intense laser field interacts with the electronic charge distribution of the atom. In addition to transferring energy to the electronic cloud of the atom, the possibility also exists for energy transfer between near-lying excited states of the nucleus. In general, the energy transfer could proceed directly from the laser to the nucleus, or indirectly via non-radiative energy transfer from the electronic motions to nuclear excitations.

Experiments show that the possibility for nuclear excitations exists due to transitions of atomic electrons to inner-shell vacancies. Additionally, laser driven excitation of the first excited state of ^{235}U has been reported (Ref. 1) and a second experiment is ongoing (Ref. 2). These experiments show the possibility of exciting ultra-low energy nuclear transitions from a nuclear ground state of possible interest in isotope separation or generating controlled gamma emissions from excited isomeric levels, by transition from long- to shorter-lived states.

In 1985, Baldwin, Biedenharn, Rinker, and Solem (Los Alamos, Ref. 3), addressed the energy transfer problem by focusing on the laser-electron interaction with a perturbative approach (Ref. 4) to estimate nuclear excitation probabilities. Alternately, Noid, Hartmann and Koszykowski (Oak Ridge, Ref. 5) proposed a study of the coupled dynamics of the system in a semiclassical approach. This work initially looked at the electron-nucleus system and, in continuation at Oak Ridge National Laboratory, has now looked at a simple model containing electron-nucleus-laser terms. Recently, Berger, Gogny, and Weiss (Livermore, Ref. 6) examined the physics of laser-driven classical electron motion with a perturbative approach to the nuclear matrix element.

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In this brief report we describe our method for calculating energy transfer between two coupled systems in the presence of a laser field. This semiclassical approach (Ref. 7) is one which solves Hamilton's dynamical equations of motion for the electron and nucleon from initial quantum conditions, and treats the laser field classically as an explicit function of time. This approach is one which provides a route to models which include both nuclear as well as electronic collective degrees of freedom.

MODEL

A simple model of coupled electronic and nucleonic independent particle motion is used as a first step to study energy transfer processes in the presence of a laser field. The time dependent Hamiltonian, $H(p,r,t)$ for the coupled electronic-nucleonic system is given by:

$$H(p,r,t) = H_n(p_n, r_n) + H_e(p_e, r_e) + H_c(r_e, r_n) + H_{\text{laser}}(r_e, r_n, t)$$

where H_n is the nuclear Hamiltonian, H_e is the electronic Hamiltonian, H_c is the electron-nuclear coupling term, and H_{laser} is the time dependent laser Hamiltonian. The nuclear Hamiltonian describes the motion of an odd proton in a Woods-Saxon well:

$$H_n(p_n, r_n) = m_n c^2 \left[\left(\frac{p_n^2}{m_n^2 c^2} + 1 \right)^{1/2} - 1 \right] + V_0 \left\{ 1 + \exp \left[\frac{(r_n - R_0)}{a_n} \right] \right\}^{-1}$$

Here m_n is the nucleon rest mass, V_0 is the Woods-Saxon well depth, a_n is the well diffusivity and R_0 is the nuclear radius. The electron Hamiltonian is:

$$H_e(p_e, r_e) = m_e c^2 \left[\left(\frac{p_e^2}{m_e^2 c^2} + 1 \right)^{1/2} - 1 \right] - \frac{e^2 \eta (Z - k)}{r_e}$$

and the coupling term is:

$$H_{\text{coup}} = - \frac{\eta k e^2}{|r_e - r_n|}$$

where m_e is the electron rest mass, Z is the nuclear charge, η is a screening parameter, and k is an artificial coupling parameter. With k equal to zero, the system is "uncoupled", with k is equal to one, the system is "coupled." The laser Hamiltonian is given by:

$$H_{\text{laser}}(r, t) = \mu(r) E \cos \omega t$$

This term contains the time-dependent contribution for the laser, characterized by electric field strength E and frequency ω . The quantity $\mu(r)$ is the dipole moment given by the electron-nucleon distance; the nuclear core is fixed at the origin of the coordinate system.

RESULTS

Laser terms and relativistic corrections, of particular importance to the electron's motion, have been added to the model reported previously (Ref. 5). This model still has dynamics characteristic of a generic nucleus (Blatt-Weisskopf transition rates) which provides a standard starting point. The nuclear frequencies are, however, high for nuclei of ultimate interest by two to three orders of magnitude; since the nuclear frequency sets the overall energy scale of the problem; the example which we depict here serves to illustrate the basic steps of the calculations and the qualitative conclusions.

For the case discussed in this paper $V_0 = -30$ MeV, $R_0 = 1.25$ Fm $A^{1/3} = 8.66$ Fm for $A=208$, $a_n = 0.65$ Fm, $Z = 82$, $m_e = 0.511$ MeV and $m_n = 938$ MeV. These are reasonable parameters for an odd proton outside a doubly magic core. The proton is initially in an $l=3$ state (with a nearby $l=1$ state) and, given the frequency scale set by the nucleon transition, the electron is started in the K state for purposes of illustration. The frequency is in units of inverse time units, where one time unit is the time for light to travel one Fermi. The frequency is converted to energy units of MeV by multiplying by 197. The electric field has units of $\text{MeV}^{1/2}$ Fm $^{3/2}$. In these convenient units $e^2 = 1.44$ MeV $\cdot$ Fm and $e^2/2\pi\hbar c$ is $1/137$.

Classical trajectories (Fig. 1) in momentum and coordinate space are generated from the Hamiltonian using Hamilton's equations: $\dot{\mathbf{p}} = -\partial H/\partial \mathbf{r}$, $\dot{\mathbf{x}} = \partial H/\partial \mathbf{p}$. The initial conditions for the trajectories are chosen from states of the separable Hamiltonian, that is, with the coupling term neglected. For each such

Fig. 1. Coupled relativistic nucleonic (radius = 8.66 Fm) and electronic (radius = 637 Fm) trajectories.

separated system, quantization of the action angle variables can, in general, include the fractional term described by Keller (Ref. 8). With the relativistic corrections though, the K orbit trajectories for Z greater than half the fine structure constant generated from initial conditions using the Langer correction (Ref. 9) are unstable. In a classical interpretation, the electrons orbit decays into the nuclear center. This behavior is associated with the singularity occurring in Sommerfeld's relativistic treatment of the Bohr atom (Ref. 10). The initial condition for the relativistic electron is thus taken to be that of the "old quantum theory" without the Langer correction. In light of the recent discussion by Jackson (Ref. 11), this is an interesting aspect to pursue.

The trajectories are used to calculate autocorrelation functions of the total system dipole moment. The absorption band shape (power spectrum) is given by the Fourier transform of the appropriate autocorrelation function. With the laser field off, the power spectrum is used to understand the basic dynamical frequencies. We find four basic frequencies in addition to the many harmonics and lower intensity frequencies. The lowest frequency of the four is associated with the orbital motion of the electron. The three higher frequencies are associated with the nucleon motion. In a crude sense, the nucleon moves in a "narrow" elliptic orbit close to the appearance of a linear vibration, this orbit precesses. The two highest frequencies arise from this "vibrational" frequency of the nucleon plus and minus half the "rotational" frequency. The rotational frequency appears between the electronic orbital and the nucleonic vibrational frequencies. When the total dipole moment autocorrelation function in the uncoupled case is transformed, components of the electronic frequency appear superimposed on the nucleonic frequencies. For the relativistic Hamiltonian (in the old quantum theory) the total dipole moment shows a stronger admixture of the electron and nucleon motion than the non-relativistic case.

The trajectory calculations with the laser term are carried out on a Cray computer at Oak Ridge National Laboratory. We integrate Hamilton's equations as a function of time for an ensemble of 64 trajectories each with a different initial phase for the laser; these phases are evenly distributed over two π radians. We choose 64 trajectories for the phase ensemble since the vector capability of the Cray allows us to run up to 64 trajectories in parallel. The explicit time dependence of the laser pulse easily allows us to vary frequency and intensity and even, if desired, the envelope.

The laser is first scanned through a range of frequencies at a fixed high intensity. For each fixed frequency, the ensemble averaged nucleon energy, electron energy and total energy are computed as a function of time (Fig. 2). Plots of the maximum energy transfer reveal resonances at which the transfer is enhanced (one such resonance is crossed in the scan shown in Fig. 2). Fourier transforms of these time dependent ensemble averages are useful in extracting frequency information on the location of significant resonances for laser absorption in the coupled system. An investigation of the intensity dependence shows that the energy transfer, largest when on a resonance, falls with decreasing electric field strength. For the case in Fig. 2, the energy transfer roughly drops by one order of magnitude for each order of magnitude decrease in the electric field strength over the range 1×10^{-6} to 1×10^{-8} ; (the intensity is proportional to the square of the electric field strength).

The energy transfer values are related to the frequency spread of the particle's motion. Typically, the ensemble energy transfer, which is related to that frequency spread, reaches a constant after some time. We have run extended time durations to verify that this ensemble frequency spread is roughly constant for an extended time duration, thus, the laser absorption is essentially a quasi-periodic function of time.

Ensemble-averaged energy as a function of time in the laser field.

Fig. 2. Time-Dependent Total Energy Transfer. The behavior of the ensemble averaged energy of the total system is depicted for six sequential values of the laser frequency from 9 to 14×10^{-4} inverse time units. Separate electron and nucleon ensembles have similar behavior with differing energy scales. On the basis of about forty such runs at differing frequencies, time durations and intensities, we study a number of such resonances.

CONCLUSION

An approach to exploring non-radiative energy transfer in coupled systems and intense laser fields has been applied to the study of energy transfer in a single-particle electron and single-particle nucleon model.

It is demonstrated that energy transfer to the nuclear motion occurs via coupling to the electronic motion in a laser field for a simplistic single-particle model of a valence nucleon and an inner shell electron at a laser resonance. Energy transfer in this system not only depends on the laser frequency but also on intensity. Electrons closest to the nucleus have greater coupling; electrons further from the nucleus though, are expected to be most affected by the laser.

The nucleon model sets the energy scale for the frequencies of the coupled system--currently this is too high for practical applications since the single-particle nucleon transitions are too high in energy. The specific features of the nucleon model can be scaled to examine lower frequency transitions and collective motions included in this approach. The electron part of the model basically describes a tightly bound electron and with suitable changes can be extended to treat outer shell electrons or collection motions (in the laser field) as appropriate.

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