

MODELING LASER STRIPPING WITH THE PYTHON ORBIT CODE

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Abstract

Laser assisted hydrogen stripping has become a widely discussed alternative to the existing stripper foil approach. A simulation tool for this new approach is presented. The application is implemented in the form of an extension module to the Python ORBIT parallel code that is under development at the SNS. The physical model in the application utilizes quantum theory to calculate the evolution and ionization of hydrogen atoms and ions affected by the superposition of electromagnetic and laser fields. The algorithm, structure, benchmark cases, and results of simulations are discussed for several existing and future accelerators.

INTRODUCTION

One of the serious problems with operating the SNS facility in Oak Ridge involves the injection system of the accumulator ring. The current system uses a thin carbon foil to convert H⁻ beam from the linac to protons at the ring injection point. The planned upgrade of SNS involves a power increase of the injected beam that will lead to excessive heating and to rapid failure of the stripper foil. For this reason SNS is developing alternative injection processes for higher powers.

There are two such investigations at SNS. The first involves the development of better stripper foils [1] and the second is the replacement of the stripper foil by a laser-assisted stripping (LS) process [2]. Moreover, LS is an attractive method for other projects using conversion-injection of H⁻ beam. This paper presents a computational model for the three step LS developed at the SNS [3-5], and that can also be applied to other projects.

Basically, the theoretical description of LS requires the self-consistent application of quantum mechanics, laser physics, and accelerator physics. The central problem is the excitation-ionization of a hydrogen beam in a superposition of electromagnetic and laser fields $H^0 + \gamma \rightarrow H^{0*} \rightarrow p + e^-$. Success of the ionization process for each particle of the beam can be predicted with probability P using quantum mechanics. The problem of LS injection is conditioned by the requirements of the total LS efficiency \bar{P} and output emittance parameters of the proton beam. By solving the problem one can determine the requirements on the input hydrogen beam and the laser beam parameters for successful injection.

The LS is a new scientific field [3-5] with no established computational component. The proof-of-principle (POP) of LS has been successfully demonstrated at the SNS [3]. To computationally support the experiment a simple quantum model [4] of adiabatic rapid passage (ARP) was applied. The model considers a two level hydrogen atom and linear frequency growth in time of the laser field in the atom's rest frame. The model consists of a system of two linear differential equations

that can be solved by any Math package. Many physical phenomena taking place in a real experiment and significantly affecting the final LS efficiency are not included in the model. Nevertheless the model yields a good estimation of LS efficiency and can be used both as an initial stage for LS calculation and for benchmarking more detailed models. It should be noted that the purpose of the POP experiments was to demonstrate feasibility of the LS idea founded on the basic principles of quantum mechanics. The expectation of the model was successfully met experimentally.

For the next experiments planned in the SNS project it is necessary to demonstrate the feasibility of LS injection for the detailed SNS requirements. Experimental LS involves many different phenomena that should be included in the calculation. These include: the Stark effect and splitting of the hydrogen atom energy levels; spontaneous decay; electric field ionization; and possible circulation of the external electromagnetic field. Computing the LS for the next experiments is necessary for determining the simplest technical equipment and for optimizing the LS efficiency over the numerous parameters in the LS scheme.

A short description of the LS physical model, taking into account all the listed phenomena, can be found in [3]. A computer model of LS presented in this paper has been realized in form of an extension module in the PyORBIT parallel code developed at the SNS [6]. The choice of the implementation is conditioned by the general direction of development of accelerator codes at the SNS. The main advantages of the chosen direction are: rapid and pure object oriented prototyping of applications at the Python level; the widespread use and detailed documentation of Python; high performance execution of the classes at the C++ level; simple writing of extension modules; and parallel computing with PyORBIT based on MPI library. Moreover the present PyORBIT already contains templates for developing extension modules. If the developer has a unique physical problem requiring different classes than those in PyORBIT, he can create new extension modules to solve the problem.

This paper is organized as follows. Section 2 gives a short overview of the physical model of the LS and formulates the mathematical problem for computing the LS. The purpose of the section is to show the amount and kinds of computations required for solving the problem of LS. Section 3 describes the organization of the LS code and classes for getting the most efficient computations. Section 4 presents benchmarks and tests of the LS code. Section 5 outlines the scope of problems that can be solved by the code. Section 6 summarizes the paper summarizing and suggests some problems to be treated in the future.

OVERVIEW OF PHYSICAL MODEL

A brief description of the complete physical model for the three step LS process can be found in [5]. The first step of LS deals with the Lorentz stripping of the H^- ion: $H^- \rightarrow H^0 + e^-$. This is a probabilistic process that can be calculated with a simple semi-empirical formula [7, 8]. This overview of physical model is devoted mainly to the second and third steps of the LS, namely the excitation and ionization of the H^0 beam. In the absence of interaction between particles, each particle of the beam can be treated independently and then the total effects of the LS can be calculated statistically.

The model assumes that after the first step of the LS process there is a hydrogen atom in the ground state with initial position and momentum $\{\mathbf{r}_0, \mathbf{p}_0\}_i$ in the laboratory frame (LF) (Fig. 1a). The atom moves under the influence of a strong high frequency laser field and a slowly oscillating external electromagnetic field.

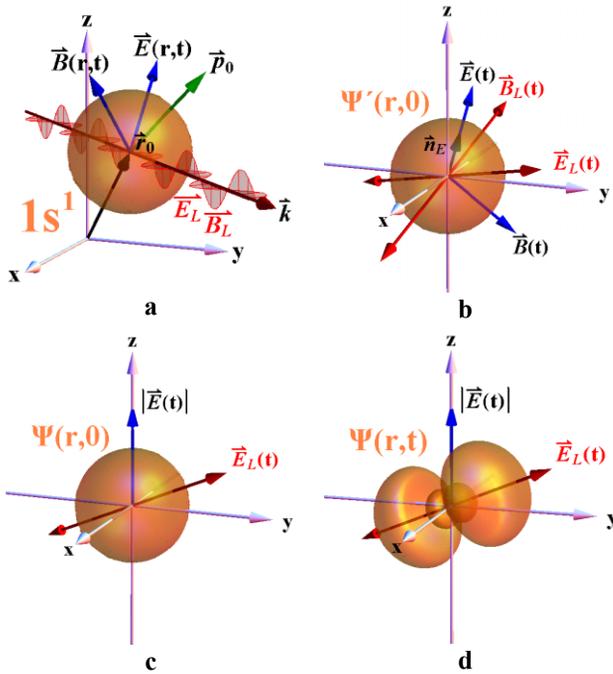


Figure 1. Schematics of a hydrogen atom in different frames considered for solving the excitation-ionization problem: **a**-laboratory frame, **b**-particle rest frame (inertial), **c**-particle rest frame (non-inertial) with z axes directed along the E field and $t=0$, **d**-the same as **c** but with $t>0$. The laser and external field vectors are shown as red and blue arrows, respectively. The orange figure represents the electron cloud of the atom.

The state of the atom travelling in the superposed electromagnetic and laser fields evolves. The problem is to find the probability of ionization of the hydrogen atom as a function of time. The state functions calculated for each H^0 particle will determine the further evolution of the beam. As a result it will be possible to calculate emittance parameters and currents of the H^0 , p, and e^- beams. The evolution of the hydrogen atom implies evolution of the electron wave function in the atom

$\Psi(\mathbf{r}, t)$. The probability of ionization of the H^0 atom can be calculated via the wave function by the following expression: $p(t) = 1 - \int \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)d^3r$.

The quantum problem for the hydrogen atom is solved in the particle rest frame (PRF). A first step is to Lorentz transform the fields and time from the LF (Fig. 1a) to the PRF (Fig. 1b). Theoretically, it is possible to solve the quantum problem in the new frame using either of two approaches: application of the Schrödinger equation (SE) for the wave function or application of the master equation (ME) for the density matrix (DM). The first method does not take into account the phenomenon of spontaneous decay but the second one does. In other respects, both methods equally well solve the problem of the hydrogen atom in the superposition of laser and external electromagnetic fields taking into account the Stark effect and field ionization.

The SE in the inertial frame (Fig. 1 b) can be written in the following form:

$$i\hbar \frac{\partial \Psi}{\partial t} = (\hat{H}_0 + \hat{H}_{E,B} + \hat{V}(t))\Psi \quad (1)$$

Here \hat{H}_0 - operator of the unperturbed hydrogen atom, $\hat{H}_{E,B}$ -interaction between electron and the electromagnetic field, and $\hat{V}(t)$ - interaction between electron and the laser field. In principle, equation (1) can be solved directly. However, this is a 4D partial differential equation of the second order that is difficult to solve without simplifying assumptions. All magnetic fields in the PRF can be omitted in comparison with the electric fields in determining the evolution of the atom. Next, for solving the problem it will be convenient to transform equation (1) and the electric fields into a frame where the external electric field (non laser field) is directed along the z axis (Fig. 1c). The new frame is non-inertial and equation (1) is transformed into the following:

$$i\hbar \left(\frac{\partial \Psi}{\partial t} + \vec{\nabla} \Psi \cdot \left\{ \frac{\partial \mathbf{M}}{\partial \mathbf{n}_E} \cdot [\vec{\omega}_E \times \mathbf{n}_E] \right\} \mathbf{M}^{-1} \vec{r} \right) = (\hat{H}_0 + \hat{H}_{E,B} + \hat{V}(t))\Psi \quad (2)$$

Here $\mathbf{M}=\mathbf{M}(\mathbf{n}_E)$ is a transformation matrix from the inertial frame \mathbf{r} (Fig.1 b) to the non inertial frame \mathbf{r}' (Fig.1 c) $\mathbf{r}'=\mathbf{M}\mathbf{r}$. If the circulation of the field in the inertial PRF is zero $\vec{\omega}_E=0$ then the new frame (Fig. 1c) is inertial and equation (2) will look like the usual SE (1). Equation (2) can be solved by the well-known method [5], [9] in which the solution $\Psi(\mathbf{r}, t)$ is represented in the form of an eigenfunction expansion:

$$\Psi(\vec{r}, t) = \sum_{n=1}^N c_n(t) \psi_n(\vec{r}) \quad (3)$$

where the $\psi_n(\mathbf{r})$ are stationary parabolic wave functions of the hydrogen atom in an electric field satisfying the equation: $(\hat{H}_0 + \hat{H}_E)\psi_n = (E_{0n} - i\Gamma_n/2)\psi_n$. Here $\hat{H}_E = -\mu_z E_z$

is the interaction operator between the electron and the external quasi-static electric field which leads to the Stark splitting of the hydrogen atom into a multi level system. In this model we assume that $E_z(t)$ is a quasi-static field not leading to atomic excitation or transitions between levels. It follows that it is necessary to solve the problem of the Stark effect prior to equation (2) and to find $E_{0n}(E_z)$, $\Gamma_n(E_z)$ and $\psi_n(E_z)$ in parabolic coordinates as functions of the field E_z .

The dependences $E_{0n}(E_z)$ and $\Gamma_n(E_z)$ were calculated numerically in the form of tables by the method described in [10] for E_z in the range between 0 and the threshold fields at which the level disappears. The functions $\psi_n(E_z)$ were calculated using second-order perturbation theory [11].

Substituting (3) into (2), after some manipulation we obtain a system of linear differential equations for complex parameters $c_n(t)$ that can be solved numerically by the Runge-Kutta method. Finally, the system of equations has the following form:

$$\dot{c}_m(t) = \sum_{n=1}^N c_n(t) f_{nm}(t) \quad m=1\dots N \quad (4)$$

The initial condition of the equation is the ground state of the atom at the initial instant: $c_n(t_0) = \delta_{1n}$. The functions $f_{nm}(t)$ contain parameters of the hydrogen atom (Stark parameters and wave functions) and the laser field. The number of equations, N , is defined by the number of hydrogen levels involved in the problem. Each level with the principal quantum number n has n^2 Stark sublevels. If we consider the excitation of n^{th} level then we should include $N=1^2+2^2+\dots+n^2 = n(1+n)(1+2n)/6$ levels into equations (3) and (4).

The DM formalism is another approach for solving the problem that takes spontaneous decay into account. DM elements for the wave function (3) $\rho_{nm}(t) = c_n(t)c_m^*(t)$, $n, m=1\dots N$ define the state of the quantum system and the wave function (3). The ME for evolution of the density matrix can be obtained similar to the SE. Finally, the system of differential equations for the DM elements has the following form:

$$\dot{\rho}_{nm}(t) = \sum_{k=1}^N [\rho_{km}(t)a_{knm}(t) + \rho_{nk}(t)b_{knm}(t)] \quad (5)$$

$$n, m = 1\dots N$$

with the initial conditions defined by the ground state of the atom at the initial instant: $\rho_{nm}(t_0) = \delta_{1n}\delta_{1m}$. The DM elements are complex and satisfy the relation $\rho_{nm}(t_0) = \rho_{mn}^*(t_0)$. Functions $a_{knm}(t)$ and $b_{knm}(t)$, similar to (4), contain the parameters of the hydrogen atom and laser field. The ME is bigger then the SE by a factor of N and consists of $N^2 = (n(1+n)(1+2n)/6)^2$ differential equations, as can be seen by comparing Eqs. (4) and (5). If we consider the excitation of the $n=3$ level, then it will be necessary to solve a system of 196 differential equations for complex elements of DM.

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After solving the equations (4) or (5) it is easy to calculate the function of ionization probability. Substituting (3) into the definition of the ionization probability we obtain:

$$p(t) = 1 - \sum_{n=1}^N c_n(t)c_n^*(t) = 1 - \sum_{n=1}^N \rho_{nn}(t) \quad (6)$$

The quantum mechanical model of LS described above covers many phenomena, excluding spin-orbital interaction and fine structure splitting. However the question of the applicability of the model and code for the calculation of LS in extremely strong external electromagnetic fields requires special consideration. In this case, perturbation theory can yield incorrect wave functions. For correct solution of the SE (1) or (2) it is necessary to take into account continuum spectra in the quantum problem without using perturbation theory.

COMPUTER CODE

The code consists of many classes responsible for different functions. This section reviews the basic classes.

Laser field

This class provides the components of the electric and magnetic laser field as a function of particle coordinates and time in the laboratory frame (Fig. 1a). Most laser beams can be well approximated by the elliptical Gaussian mode [12]. In the LS problem the components of the laser field are represented in a complex form for simplification of mathematical equations and the code:

$$E(x, y, z, t) = \frac{2\sqrt{cPw_xw_y}}{\pi\sqrt{h_xh_y}} e^{ik(ct-z) - \frac{x^2}{h_x} - \frac{y^2}{h_y}} \quad (7)$$

$$h_{x,y} = w_{x,y}^2 - \frac{2i(z - f_{x,y})}{k}$$

where $k=2\pi/\lambda$, P is the power of the beam and c is the speed of light. The magnetic field B can be written as $B=E/c$. The elliptical Gaussian laser beam (7) is specified by four geometrical parameters: w_x, w_y – horizontal and vertical waists, and f_x, f_y – positions of the waists.

In general, the result of the interaction of a particle beam with the laser beam depends on the local characteristics of the laser beam at the point of interaction. For this reason, it is convenient to operate with r_x, r_y – sizes of the beam and α_x, α_y – angles of divergence of the beam at this point. The local parameters can be expressed mathematically using the first four parameters.

The expression (7) defines a continuum laser beam. For the next LS experiments at the SNS a pulsed laser source ($\tau \sim 50$ ps, $\lambda=355$ nm) will be used. Because this is not an ultrashort laser pulse, the temporal shape of the laser power P in (7) can be described by a Gaussian function: $\exp[-4 \cdot \text{Ln}(2) \cdot (t-z/c)^2/\tau^2]$. Here τ is the full width at half-

maximum FWHM. The electric field (7) should be multiplied by the square root of this function.

Stark effect

This class provides Stark parameters for equations (3) and (4) as functions of the electric field. These functions have been calculated previously by another code and stored as data files. The energy E_{0n} and lifetime⁻¹ Γ_n are stored in the form of numerical functions and the dipole transitions $\mathbf{d}_{nm} = \int \psi_n^*(\mathbf{r}) \mathbf{e} \psi_m(\mathbf{r}) d^3r$ are stored as coefficients of the power series expansion $\mathbf{d}_{nm}(E_z) = \mathbf{d}_0 + \mathbf{d}_1 E_z + \mathbf{d}_2 E_z^2$.

A resonant phenomenon occurring at the interaction of the laser field and the atom significantly affects the efficiency of LS. This phenomenon, mathematically contained in equations (3) and (4), strongly depends on the precision of the energies $E_{0n}(E_z)$. For this reason, the more exact method [10] was used for computation of the energies. For computation of the dipole transitions playing a minor role, the perturbation theory has been applied.

Two level atom

This is a class for computation of laser stripping based on the SE or ME when only two levels $N=2$ are included in the series expansion (3). The two level atom model for the interaction of light with matter leads to the system (4) consisting of two equations. Practically, the approach is valid only when: no external static field is applied to the atom; the electric field is directed along the z axis in the PRF (Fig 1.c); and the eigenfunctions (3) are expressed in spherical coordinates. In other words, the class can be applied for computation of LS without external static electric fields in the PRF and for linearly polarized laser fields. From the point of view of computing, this is a high performance class that can be used for initial estimations of LS.

Schrödinger equation

This class performs the calculation using the SE approach described in the previous section. It takes into account everything except spontaneous decay from upper to lower levels. Nevertheless the class can be used for the calculation of LS in the presence of external quasi-static fields for atoms having small time of interaction with laser field. The validity of the computation requires a negligible spontaneous decay rate, or small evolution times in contrast with lifetime of an exited atom. Practically, this is the best class when considering the performance-potentialities relationship, and it is useful for optimization of the laser and external field parameters.

Density matrix

This class is based on the DM approach described in the previous section. Although the method includes many phenomena, it is computationally too slow to be used for optimization requiring multiple computations. Practically, the method can be used for the final calculation of LS efficiency after optimization by the SE method.

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Diagonal density matrix

In the absence of laser fields the master equation (5) is modified such that the equations for the diagonal elements $\rho_{nn}(t)$ are separated from those for nondiagonal elements. As a result we obtain system of N linear differential equations for the diagonal elements of DM:

$$\dot{\rho}_{nn}(t) = \sum_{k=1}^N \rho_{kk}(t) f_{kn}(t) \quad n=1\dots N \quad (8)$$

This class, as well as the previous class, can be applied for computation of LS after calculation by the SE method. However in contrast to the previous class for calculating the 2nd and the 3rd steps of the LS this class calculates only the 3rd step and has much faster performance then the previous one. This class, in combination with (6), is very useful for the computation of emittance growth of stripped atoms, which can be very important for some projects. The derivative of (6) $\partial p(t)/\partial t$ gives the spatial distribution of the current density of stripped atoms. The density is nonzero only in the presence of transverse magnetic field in the LF. The space distribution leads to the spread of trajectories of the stripped particles in the magnetic field and to emittance growth.

Another important application of the class is for computation of beam losses during foil stripping. In this case the beam loss is due to the few percent of partially stripped beam that remains neutral H^0 after passing through the foil. The empirical distribution of the initial exited states $\rho_{nn}(t_0)=f(n)$ of the neutral beam can be found in [13]. After applying this class it is possible to calculate the evolution of the beam and its losses.

A similar thing can be done for LS. The initial distribution of exited states of the H^0 beam $\rho_{nn}(t_0)=f(n)$ can be written analytically without numerical simulations and the class can be applied to compute losses and emittance growth due to LS.

Ionization of H^- beam

This class calculates the stripping of H^- beam travelling in external electromagnetic fields. This is the first step of the LS. In this case only one state of the ion is possible. The system of equations (8) is transformed into the single equation:

$$\dot{\rho}_{11}(t) = -\Gamma(E(t))\rho_{11}(t) \quad (9)$$

with the condition $\rho_{11}(t_0) = 1$. The empirical dependence $\Gamma(E)$ for the H^- ion can be found in [7, 8].

BENCHMARKS

This section presents benchmarks of the LS code based on: fulfilment of quantum mechanical laws; comparison of the classes with each other; and checking the results of computation with a simple analytical case. Let us begin with a particular case that can be calculated analytically. This method was applied for checking the two-level

model [4]. Let the electric component of the laser field in the PRF have the following form:

$$\vec{E}(t) = \vec{E}_0 e^{i\left(\omega_0 t + \frac{\Gamma t^2}{2}\right)} \quad (10)$$

where ω_0 is a resonant frequency between the 1st and the 2nd level of hydrogen. Assume that the frequency of the laser field grows linearly with time, passing through resonance at $t=0$: $\omega(t) = \omega_0 + \Gamma t$. We direct the field \vec{E}_0 along z axes and after calculation we obtain the following evolution of the 1s and 2p states in the spherical basis (Fig 2). The population of the upper state (2p-state) calculated in our case as $|c_{2p}|^2$ can be predicted analytically [4] at $t \rightarrow \infty$. The numerical results are in good agreement with the analytical formula.

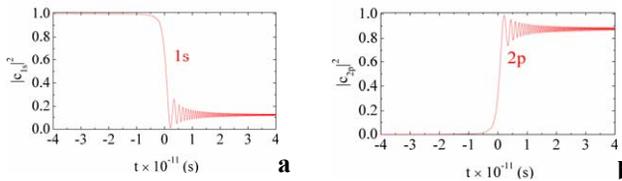


Figure 2. Evolution of populations of 1s-2p states of a hydrogen atom in a benchmark laser field.

The result should not depend on the coordinates we use to solve the problem, spherical or parabolic. Let us direct vector \vec{E}_0 in (6) along $\mathbf{n} = \{1, 1, 1\}$ direction for generality and solve the problem in parabolic coordinates by the SE. Then we obtain the following picture (Fig 3.) that shows that the evolution in the parabolic basis matches the evolution in the spherical basis (Fig. 2a).

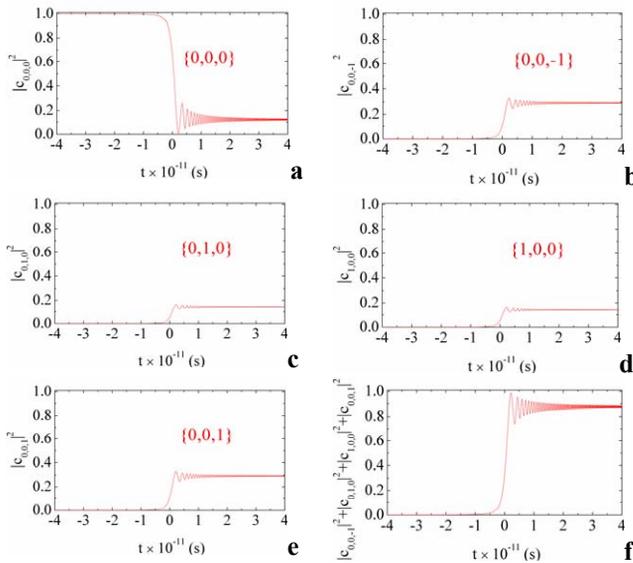


Figure 3. Evolution of populations of parabolic states with principal quantum numbers $n=1, 2$ for hydrogen atom.

The sum of the populations of the 2nd states in the parabolic basis shown in Fig. 3f matches the population

of the 2p state in the spherical basis (Fig. 2b). If we exclude spontaneous decay from ME and solve Eq. (5), then we obtain exactly the same results shown in Fig. 3 for the diagonal elements of DM. As expected, the results are matching because equation (5) follows directly from (4) when spontaneous decay in (5) is omitted. The sum of all populations is 1 for all 3 methods.

If we set $\Gamma=0$ in (10), then the atom will be affected by the resonant frequency ω_0 and we will observe Rabi oscillations. These can be also described analytically and shown to match for all the methods. In this way, we tested different classes and found them to be in agreement with the basic principles of quantum mechanics, with the analytical formulas, and with each other.

Another instructive example is a computation of the atom evolution in an external static electric field while applying the same laser field (10). The result of the calculation is shown in Fig. 4, both for the SE and the ME. One can see that the different parabolic states with different energies will be excited in different moments of time. This happens due to resonance physics of the excitation process and the linearly changing frequency of the laser field.

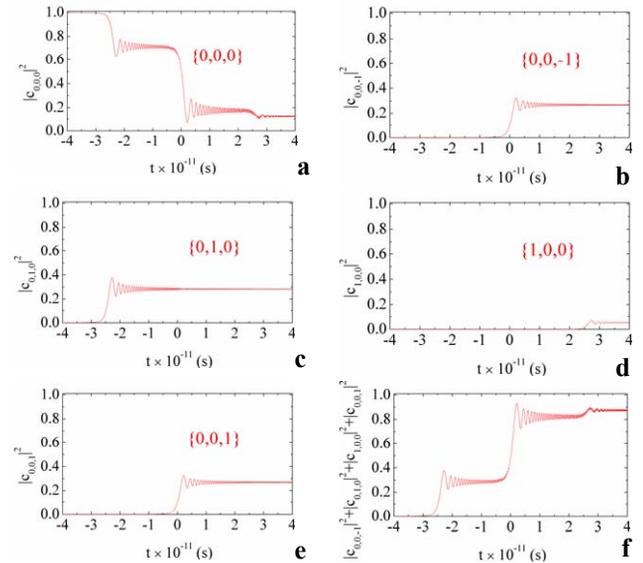


Figure 4. Evolution of populations of parabolic states with principal quantum numbers $n=1, 2$ in the presence of an electric field directed along the z axis.

This picture corresponds to the realistic LS excitation by the laser field (7) showing behaviour similarly (10) in the PRF and realizing the idea of the ARP.

APPLICATIONS OF THE CODE

The purpose of the code is the optimization of laser stripping systems. Below we list only a few of the questions that can be resolved using these models. One of the main technological problems of LS is getting a high efficiency while using a relatively low power laser. Let us consider the LS scheme with a single pass laser beam (7). The parameters $r_x, r_y, \alpha_x, \alpha_y$ of the beam can be optically

adjusted. The optimization of these parameters can be easily realized using the code together with an optimization package.

Another problem is the possible modification of the temporal shape of the laser pulse, which can become very important for LS. A laser micropulse with a given peak power and FWHM can be extremely non-optimized for stripping of a hydrogen beam with given FWHM. In this case it is reasonable to try to modify the laser micropulse shape while conserving the pulse energy. The LS code can provide parameters of the laser pulse optimized for best LS efficiency.

In most cases, σ – the polarization of the laser field in the PRF, provides better LS efficiency in contrast with π - polarization because of less Stark splitting of energies ΔE_n of excited states. In any particular case, questions about polarization can be resolved with the code.

The three step LS scheme for intermediate experiments at the SNS is shown in Fig. 5. Two dipole magnets of opposite polarities provide stripping of the first and the second electrons. The magnetic field in the region of interaction between the magnets is minimal and can be described by formula $\mathbf{B} = C(x\mathbf{e}_z + z\mathbf{e}_x)$ where C (T/m) is obtained from the distance between the magnets and their strength.

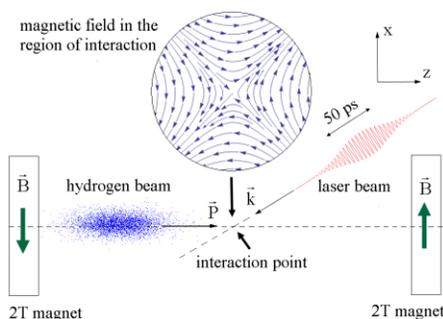


Figure 5. Schematics of laser stripping for the SNS.

Using the code it is possible to optimize the distance between the magnets. On the one hand, increasing the distance between the magnets decreases the field strength in the interaction region. This leads to a decrease of perturbation of the atom, less Stark effect, and improvement of the resonant excitation and LS efficiency. On the other hand, greater distance between the magnets leads to longer travel times of excited atoms from the interaction point to the second magnet. This circumstance increases the effect of spontaneous decay and decreases total LS efficiency. From the point of view of the code the distance between the magnets can be considered as a parameter that can be optimized.

Computations for the next LS experiments at the SNS conclude that it is possible to obtain 90% of LS excitation using a single pass laser micropulse with 2 MW peak power and 50 ps FWHM in time. The H^0 beam is considered to have the same temporal FWHM and given parameters of emittance. More details about the estimations can be found in [14].

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SUMMARY

- A new code for the calculation of the three-step laser assisted stripping of H^- beams has been developed.
- The computational model was implemented as an extension module for the PyORBIT parallel code developed at the SNS.
- Benchmarks of the code demonstrate its reliability and confirm its correspondence with the mathematical model and with the basic principles of quantum mechanics.
- The code was used for optimizing the laser stripping experiments for the SNS project.
- In the future it will be necessary to perform theoretical investigations on the excitation of hydrogen atoms in a strong static field. It will then be necessary to include continuum spectra into the quantum mechanical problem.

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