

PHYSICAL MODEL OF HYDROGEN ION LASER STRIPPING*

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Abstract

Thin carbon foils used as a charge strippers for H^- ions have a limited life time and produce uncontrolled beam loss. Thus, foil based injection is one of the factors limiting beam power in high intensity proton rings. There is a possibility to replace such foils by laser-assisted stripping of negative hydrogen ions, a method developed and demonstrated at the SNS accelerator in Oak Ridge. In this paper we present progress in the physics and computation of H^- laser stripping. We present a physical model which includes such factors as the Stark effect, the polarization of the laser field, and the spontaneous relaxation and autoionization of hydrogen atoms in a strong electro-magnetic field. The model formulates a quantum mechanical problem that can be solved numerically using a module created for the PyORBIT parallel code developed at SNS.

INTRODUCTION

The future power upgrade of the SNS accelerator [1] faces challenges related to the existing foil based ring injection. Currently, thin carbon foils provide conversion of H^- ions to the protons beam for injection into the ring. Problems can arise when high average beam currents pass through the foil. This can lead to a shorter lifetime of the foil, higher absolute beam losses, and facility activation. These shortcomings complicate the maintenance, and are considered to be a very serious factor for multi-MW proton facilities of future. Similar problems are also expected to show up in other projects [2].

Recently, laser assisted stripping of H^- ion beam (LS) has attracted attention [2] as a good alternative to stripping foils. The proof-of-principle of the LS has been successfully demonstrated at SNS in Oak Ridge [3]. The next experimental steps [2] require a physical model that includes all factors and phenomena affecting the final LS efficiency. This model is also necessary for optimization of the LS installation. In this paper we present such a model and the computational results for the SNS project.

The excitation of H^0 hydrogen atoms from the ground state to the upper states by the laser beam is the most critical and theoretically complicated part of LS, defining efficiency of LS in general. In the theoretical investigation [4] that has become a foundation for the proof-of-principle experiments [3], the hydrogen atom is presented as a non perturbed (1s-3p) two-level atom. A laser field for numerical estimations was presented as a round Gaussian beam. For the H^0 beam, the realistic SNS emittance [5] was used. The proof-of-principle experiment confirmed the validity of this model.

The LS setup for the next experimental step includes two strong dipole magnets for Lorenz stripping of two

electrons. Hence, laser excitation of the H^0 beam located between these magnets is affected by the magnetic field and the Stark effect taking place in a particle rest frame (PRF), and should be included in the model of LS. The calculation of the energy levels and the lifetime of the hydrogen atom in a strong electric field is a difficult theoretical problem itself. For the Stark effect calculations we used a numerical approach found in references [6, 7].

Exited atoms travelling after the excitation are affected by spontaneous emission. If emission occurs, atoms will not be stripped of their electrons and will be lost from the injection process. This loss will reduce the total efficiency of LS and should be included in the model for further optimization.

Another improvement of the LS physical model [2] is a more realistic description of the laser beam. The initial model assumed a round Gaussian laser beam which is not expected to be present in future experiments. The real laser beam consists of an infinite number of modes including an elliptical Gaussian mode which makes up the most of the beam.

Finally, the new physical model has been implemented as a module in the PyORBIT parallel code. The Python programming language driving shell allows a fast estimation and optimization of the LS efficiency for different parameters and features of a given LS scheme.

In this paper we will present the description of the physical model of LS including the effects listed above. We will also discuss several examples of computations for the SNS project with a new application.

PROBLEM DEFINITION

According to the three-step scheme of LS [4], the first stripping magnet provides conversion of an H^- beam to an H^0 beam. As a result, we have H^0 ground-state beam that has to be excited in the second step. Omitting the first step we consider the H^0 beam as the initial condition of the subsequent problem of finding the LS efficiency related to steps 2 and 3. The problem can be formulated in the following way: We need to find the probabilities of ionisation $H^0 \rightarrow p+e^-$ as a function of time $p_i(t)$ for i -th particle of the beam travelling through the superposition of static electric and laser fields. The functions allow calculating the number of protons and their initial conditions $\{\mathbf{r}_0, \mathbf{p}_0\}_i$. The ratio of the number of protons to the number of initial H^0 atoms yields the total LS efficiency. Thus, we can calculate ring injection process.

To solve this problem, consider the evolution of quasi stationary wave functions $\Psi(\mathbf{r}, t)$ of the electron in the PRF of i -th hydrogen atom. The wave function of the atom can be found independently for each atom and then used to calculate the probability function: $p(t) = 1 - \int \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)d^3r$. The solution $\Psi(\mathbf{r}, t)$ can be presented in the form of an eigenfunction expansion:

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

where N is the number of states of the hydrogen atom involved in the dynamics.

The atom travelling in a static transverse magnetic field in the laboratory frame is affected by a static electric field in the PRF. We use the quasi-stationary wave functions of the H^0 atom in the electric field as eigenfunctions for (1). Thus, we should solve the Stark effect problem first and then find the eigenfunctions $\psi_n(\mathbf{r})$ and complex eigenenergies $E_n = E_{0n} - i\Gamma_n/2$ [6, 7] as functions of the electric field E . It should be noted that we included the time factors $\exp[-i(E_{0n} - i\Gamma_n/2)t/\hbar]$ of the stationary states ψ_n in the coefficients $c_n(t)$. For solving the Stark effect problem it is required that z-axis of the PRF to be parallel to the electric field.

The amplitudes $c_n(t)$ in (1) evolve depending on the laser field. According to the initial condition mentioned above, we should assume that $c_n(t_0) = \delta_{1n}$, because $\psi_1(\mathbf{r})$ is the wave function of the ground state. It is enough to include in (1) only states with real energies E_n satisfying $E_n - E_1 \lesssim \omega\hbar$ where ω is the laser frequency in the PRF. The validity of the reduction is conditioned by the resonance process (which can be shown mathematically). The resonant process allows exciting only upper states $\psi_1(\mathbf{r}) \rightarrow \psi_n(\mathbf{r})$ with energies $E_n - E_1 \approx \omega\hbar$ that spontaneously decay further into lower states $\psi_n(\mathbf{r}) \rightarrow \psi_k(\mathbf{r})$ with energies $E_k < E_n$. For example, if we excite the 3rd energy level of hydrogen atom then we should include $N = 1^2 + 2^2 + 3^2 = 14$ Stark states into (1).

To find the wave function $\Psi(\mathbf{r}, t)$ we need to find $c_n(t)$ by using different approaches which depend on the requirements of the particular problem. There are two equations that can be applied.

SCHRODINGER EQUATION

It is known that the phenomena of spontaneous emission cannot be included within the framework of the Schrodinger equation (SE). Nevertheless, the SE can be applied in cases where the spontaneous decay time is much longer than the time of the atoms interaction with the laser field. Then, the SE can be used to estimate the efficiency of the excitation. The SE for H^0 atom in the PRF can be written as:

$$i\hbar \frac{\partial \Psi}{\partial t} = (\hat{H}_E + \hat{V}(t))\Psi \quad (2)$$

where $\hat{H}_E = \hat{H}_0 - \mu_z E_z$ is the Hamiltonian of the hydrogen atom in a uniform electric field $\mathbf{E} = E_z \hat{\mathbf{e}}_z$ directed along the z-axis and $\hat{V}(t) = -\boldsymbol{\mu} \cdot \mathbf{E}(t)$ represents the interaction between an electron with a dipole moment $\boldsymbol{\mu} = q\mathbf{r}$ and the laser field $\mathbf{E}(t)$. Applying a well known method [8] to solve the equation (2) and recalling that $\hat{H}_E \psi_n = (E_{0n} - i\Gamma_n/2)\psi_n$, we obtain a system of differential equations for $c_n(t)$:

$$i\hbar \dot{c}_m = \sum_{n=1}^N V_{mn}(t) c_n + c_m \left(E_{0m} - \frac{i\Gamma_m}{2} \right) \quad (3)$$

where $V_{mn}(t) = \int \psi_m^*(\mathbf{r}) \hat{V}(t) \psi_n(\mathbf{r}) d^3r$. It is difficult to compute the equations (3) directly because of the high frequency of oscillation of the $c_n(t)$ coefficients. The final system of equations can be obtained using a change of variables $c_n(t) = a_n(t) \exp[-iE_{0n}t/\hbar]$, presenting the laser field in a complex form and applying the rotating wave approximation, thereby neglecting of rapidly oscillating terms in the sum.

The LS project at SNS in Oak Ridge aims to use the 3rd energy level for the laser excitation. The time of interaction of the 1 GeV hydrogen beam with the laser field located in 1 mm region is approximately 10^{-12} sec which is much less than a typical time of a spontaneous decay $\tau_{3p \rightarrow 1s} = 6.1 \times 10^{-9}$ sec. In this case the SE can be applied to the computation of the excitation efficiency.

MASTER EQUATION

After excitation the beam travels a distance of 10-20 cm through the second stripping magnet (the 3rd step of LS). In this step the efficiency of LS will be reduced by a few percent due to spontaneous decay. For this part of the LS the density matrix formalism can be applied.

The density operator for the hydrogen atom described by the wave function (1) can be written as $\hat{\rho} = |\Psi\rangle\langle\Psi|$. A calculation of the density matrix (DM) elements yield: $\rho_{nm}(t) = \langle \psi_n | \hat{\rho} | \psi_m \rangle = c_n(t) c_m^*(t)$. The DM completely defines the state of the Hydrogen atom. Substituting (1) into the definition of the ionization probability function we obtain,

$$p(t) = 1 - \sum_n c_n(t) c_n^*(t) = 1 - \sum_n \rho_{nn}(t) \quad (4)$$

The evolution of the density operator obeys the equation:

$$i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}] - \frac{1}{2} i\{\Gamma, \hat{\rho}\} + D\{\hat{\rho}\} \quad (5)$$

where the curly brackets denote an anti-commutator, and Γ is an operator of autoionization with matrix elements $\Gamma_{nm} = \delta_{nm}\Gamma_n$. The operator $D\{\hat{\rho}\}$ is a dissipation operator responsible for spontaneous transitions. The equation for the DM elements $\rho_{nm}(t)$ is called the Master Equation (ME), and can be obtained via equation (5). In the case of a non-degenerate system (a hydrogen atom in an electric field) it is permissible to use the Pauli form of the $D\{\hat{\rho}\}$ operator in combination with parabolic Stark eigenstates $\psi_n(\mathbf{r})$. It should be noted that the Pauli form is not valid for the degenerate system (an unperturbed hydrogen atom) in combination with parabolic eigenstates $\psi_n(\mathbf{r})$ [9].

If the SE was used prior to the ME for calculation of the same hydrogen atom then the initial condition for the

DM can be easily obtained from the solution of the SE: $\rho_{nm}(t_0) = c_n(t_0)c_m^*(t_0)$. The ME can also be used for calculations of complete dynamics of the hydrogen atom including steps 2 and 3, beginning from the ground state. In this case $\rho_{nm}(t_0) = \delta_{1n}\delta_{1m}$.

The main reason to avoid using the ME where possible is the long computation time compared with the SE and the two-level model [4]. For example, computation of LS with excitation of the 3rd energy level of an atom requires including 14 Stark levels into the problem. In turn, it leads to a system of $14 \times 14 = 196$ equations using the ME whereas using the SE and the two-level model leads a system of 14 and 2 equations correspondingly.

SIMULATION PACKAGE

For the computation of the Stark effect a separate computer application was created. The application uses the method of Breit-Wigner parametrization [6] to provide a high degree of accuracy for complex eigenvalues at moderate fields. For calculations of eigenfunctions a first order perturbation theory [10] was applied. For the strong fields needed for Lorentz stripping of the second electron it is necessary to use an exact numerical solution [7] based on the original definition [8] of the complex eigenvalues and quasi-stationary eigenfunctions.

The application for the computation of LS was developed as an extension to the PyORBIT parallel code [11].

SOME CALCULATIONS FOR THE SNS

We now present calculations for the laser beam recirculation scheme proposed in [12]. A realistic laser beam was approximated by an elliptical Gaussian mode [13]. The emittance of the initial H⁰ beam was taken from [5]. The angle of incidence between the laser beam with wavelength $\lambda = 355$ nm and the H⁰ beam with energy $T = 1$ GeV was set to provide the exact resonance excitation of the 3p level without external fields. Numerical investigations have shown that the efficiency of excitation grows proportional to the distance between the waste of laser beam and the interaction point. The designed geometry of the recirculation scheme [2] does not allow the distance to be more than 20 cm.

The first problem was to find the optimized parameters of the laser beam (w_x, w_y -wastes) to provide the best and most stable efficiency in a wide range of laser powers, from 1 to 10 MW. The optimization yielded $w_x = 90$ μ and $w_y = 1100$ μ , with efficiency of excitation from 78-98%.

Another important problem is the influence of the magnetic field strength on the efficiency. Calculations have shown that the transverse magnetic field $B \approx 0.005$ T reduces the efficiency by $\approx 1\%$. However, in the LS of SNS the magnetic field is created by two stripping dipole magnets with opposite polarities. Computation of the magnetic field with the ANSYS package has shown a good quadrupole field $B = C(y\hat{e}_x + z\hat{e}_y)$ in a large region near excitation point of the H⁰ beam. Calculations of the

efficiency of LS have shown that the quadrupole field with $C \approx 1$ T/m reduces the efficiency by $\approx 1\%$.

The tolerances of the H⁰ beam emittance parameters were also investigated and found to be in accordance with experimental expectation.

CONCLUSIONS

- An adequate physical model for the laser stripping including numerous atomic phenomena is developed.
- A computer model has been implemented as an extension module to the PyORBIT parallel code.
- A preliminary set of calculations for the SNS laser stripping have been completed.
- In the future, for exact calculations of the 3rd step it will be necessary to use a more exact numerical method for computation of the Stark parameters.
- In the present time the equations of quantum mechanics consider a constant direction of the static field in the particle rest frame. In the future "centripetal" operator terms for a circulating field should be included into the equations.
- For possible calculations of laser stripping in a superposition of a laser field and a strong static field it is necessary to include continuum spectra and the broadening of Stark levels into the equation of quantum mechanical equations.

REFERENCES

- [1] J. Galambos, "Progress with MW-Class Operation of the SNS", this conference.
- [2] Mini-Workshop on Laser Assisted H⁻ Beam stripping, Oak Ridge, February 2009. <http://wiki.ornl.gov/events/lahbsa/default.aspx>.
- [3] V. Danilov, et al, PRSTAB, 10, 5 (2007) 053501.
- [4] V. Danilov, et al, PRSTAB, 6, (2003) 053501.
- [5] A. Aleksandrov, et al, "Experimental setup of intermediate SNS laser stripping project", SNS Tech Note 176, 2007. <http://it.sns.ornl.gov/cgi-bin/asd/note1LinePrint>.
- [6] R. J. Damburg and V. V. Kolosov, J. Phys. B 9, 3149 (1976); "Rydberg states of Atoms and molecules", edited by R. F. Stebbings, Cambridge University Press, (1983).
- [7] V. V. Kolosov, J. Phys. B 20, 2359 (1987).
- [8] L. D. Landau and E. M. Lifshitz, Quantum Mechanics, 2nd ed. (Pergamon, New York, 1978).
- [9] D. B. Uskov and R. H. Pratt, J. Phys. B 37, 4259 (2004).
- [10] A. A. Kamenski and V. D. Ovsianikov, J. Phys. B 33, 491 (2000).
- [11] A. P. Shishlo et al, ICAP'06, Chamonix, France, October 2006, p. 219 (2006).
- [12] I. Jovanovich et al, PAC'07, Albuquerque, New Mexico, June 2007, p. 1251 (2007).
- [13] T. Freearge, J. Coutts, J. Walz, D. Leibfried and T. W. Hänsch, J. Opt. Soc. Am. B 14, 2010 (1997).