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Lorentz Dissociation of H ions in a Cyclotron

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Abstract: Stripping extraction of hydrogen ions has gained growing interest in cyclotron industry due to its high extraction efficiency. However, accelerating hydrogen anion/molecular ions experience a continuous magnetic field, further results in undesired Lorentz dissociation during acceleration. Past study of Lorentz dissociation under electric field comparable to the one in a typical cyclotron (a few MV/cm) are sparse and scattered. Hence, in order to fill in the missing yet crucial information when designing a cyclotron, this work compiles and summarizes the study of Lorentz dissociation of H⁻, H₂⁺ and H₃⁺ for stripping extraction in a cyclotron.

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1 Introduction

Stripping extraction takes away one or more electrons from the accelerated particles by passing them through a thin stripper foil located at the desired extraction position. As the stripped particles usually have different chargeto-mass ratios, the stripped ions are deflected away from the original orbit, leading to nearly 100% of extraction efficiency [\[1,](#page-14-0) [2\]](#page-14-1). This appealing feature causes it to gain a lot of interest, especially in the production of a high intensity proton beam. TRIUMF is among the biggest cyclotron that adopted the H[−] extraction [\[3\]](#page-14-2), while the DAE δ ALUS Superconducting Ring Cyclotron [\[4\]](#page-14-3) and the TR150 cyclotron proposed by Yi-Nong et. al. (it is published somewhere in this issue) are the latest projects that adopted the extraction of H_2^+ and H_3^+ ions respectively.

Although stripping extraction has a promising extraction efficiency, there are other issues that are crucial for real practice at high power. The most important issue is the Lorentz dissociation of the accelerated ions under the continuous effect of magnetic field. This often results in beam loss that are highly undesired. Therefore, in order to look into the seriousness of this problem and to investigate the impact it has in limiting the beam intensity at different energies, this work studies and compares the Lorentz dissociation of three different hydrogen ions that are good candidates for stripping extraction: H^- , H_2^+ and H_3^+ .

2 Stripping extraction

Stripping extraction of the H^- ions is the most common and easiest among the three hydrogen ions. This is because of the exactly opposite charge states of H^+ , causing them to be naturally deflected out of the cyclotron after being stripped. An example of the trajectory of stripping extraction of H[−] is also illustrated in Figure [1a.](#page-3-0)

On the other hand, unlike the simple opposite trajectory of H[−], stripping of H_n^+ of the same sign causes the particle to immediately bend inward after stripping. This is due to a smaller mass-to-charge ratio of the stripped particles, resulting in an n times smaller radius. A more complicated beam

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dynamics is required in order to extract the stripped H^+ out of the cyclotron. For instance, Figure [1b](#page-3-0) and [1c](#page-3-0) show the trajectories of stripping extraction of H_2^+ and H_3^+ during the last turn. From the figures, the stripped protons have almost half and one-third of the initial radius of H_2^+ ions and H_3^+ ions respectively. In fact, stripping extraction of H_3^+ is better, as the former has a tendency of passing through the central regions, potentially causing undesired beam loss before being extracted from the cyclotron.

Figure 1: Sample trajectories to strip the three different types of H ions (red) in order to obtain 150 MeV/u H^+ beams. The stripper foil is indicated by the small black line. Note that B_0 is the average central magnetic field at the median plane of the cyclotron.

3 Lorentz dissociation of hydrogen ions

3.1 Equivalent electric field

From Lorentz transformation, the equivalent electric field in the rest frame of a charged particle moving with velocity \bf{v} is given by

$$
E'_{\parallel} = \frac{(\mathbf{E} + \mathbf{v} \times \mathbf{B})_{\parallel}}{\sqrt{1 - \beta^2}} \qquad E'_{\perp} = \frac{(\mathbf{E} + \mathbf{v} \times \mathbf{B})_{\perp}}{\sqrt{1 - \beta^2}} \qquad (1)
$$

where **E** and **B** are the external electric and magnetic field respectively; β is the ratio of the particle's speed, v , to the speed of light, c .

Considering only the effect in radial direction, equation [1](#page-4-0) can be simplified as:

$$
E'_{r} = \frac{E_{r} + v_{z}}{\sqrt{1 - \beta^{2}}}
$$

= $\gamma (E_{r} + v_{z})$ (2)

As contribution of $B_z \gg E_r$ in a cyclotron, we can treat equation [2](#page-4-1) as follows:

$$
E'_{r} = \gamma \beta c B_{z}
$$

\n
$$
\approx (3 \text{ MV/cm}) \gamma \beta (B_{z}/1 \text{ T})
$$
 (3)

For convenience, E'_r will be expressed simply as $\mathcal E$ in the following discussion of this work.

As
$$
\gamma = \frac{E_0 + T}{E_0}
$$

\n $= 1 + \frac{T}{E_0}$
\n $\gamma \approx 1 + \frac{A(T/n)}{A(E_{H+})}$
\n $\approx 1 + \frac{T/n}{E_{H+}}$

given T as the total kinetic energy of ions; A as the atomic mass number; E_0

as the rest mass energy of the ion; E_{H+} as the proton mass energy. If the final kinetic energy per nucleon, T/n , remains unchanged, $\gamma\beta$ and the equivalent electric field, \mathcal{E} , are similar for H⁻, H₂⁺ and H₃⁺ at the same B_z .

Figure 2: The equivalent electric field $\mathcal E$ of hydrogen ions

3.2 H[−]

H⁻ is extracted by $H^- \rightarrow H^+ + 2e^-$. Despite the simplicity and efficiency of this method, the small binding energy (about 0.7 eV) of the second electron in the H[−] ions is a potential source of beam loss during acceleration. The equivalent electric field induced within the rest mass frame of the H[−] ion causes the electrons to be stripped away during acceleration. This phenomenon is commonly known as Lorentz stripping. Due to the popularity of stripping extraction of H[−], this effect is well studied and documented by many past researches [\[5\]](#page-15-0).

In principle, the integrated fractional beam loss, F , due to Lorentz strip-

ping at a given energy can be estimated by

$$
F = 1 - f \tag{4}
$$
\n
$$
\frac{df}{ds} = -\frac{f}{\gamma \beta c \tau}
$$
\n
$$
\ln\left(\frac{f_2}{f_1}\right) = -\frac{s_2 - s_1}{\gamma \beta c \tau}
$$
\n
$$
\therefore f_2 = f_1 \exp(-\frac{\Delta s}{\gamma \beta c \tau}) \tag{5}
$$

$$
\tau = \frac{A_1}{\mathcal{E}} \exp \frac{A_2}{\mathcal{E}} \tag{6}
$$

where τ is the rest-frame life time of the H⁻ ion; A_1 and A_2 are 7.96×10^{-6} V-s/m and 4.256×10^9 V/m respectively. They are fitting constants obtained from experimental results [\[5\]](#page-15-0). f is the H⁻ fraction surviving in the beam and s is the length along the beam path.

In this estimation, f_2 is the survival fraction after travelling through one turn $\Delta s = 2\pi r_{\text{effective}}$ (assuming B is a constant, i.e. omitting any flutter). When the particle accelerates, $r_{\text{effective}}$, β and γ change and thus, f_2 changes every turn. Assuming the injection energy is negligible and the peak RF voltage is 60 kV with 8 gaps for acceleration, the energy gain per turn is 0.48 MeV. Consequently, the total fraction of dissociation over all turns are determined. This integrated fractional loss is shown in Figure [3.](#page-7-0)

From Fig. [3,](#page-7-0) F of H⁻ particles accelerated up to 1 GeV is 100% for any $B > 0.4$ T. Taking a minimal beam loss of less than 0.01% for hands on maintenance of a cyclotron, the maximum energy attainable at a low $B = 0.4$ T is about 570 MeV at about $r = 10$ m. Hence, any acceleration at high energy is uneconomic, as the average magnetic field will be too low to achieve desired beam loss, and the machine has to be extremely large to accommodate such a low B field.

To date, only TRIUMF cyclotron can accelerate H[−] to high energy region (> 400 MeV) due to the size requirement to control the Lorentz stripping. The TRIUMF cyclotron has a low average $B < 0.46$ T and a large extraction radius of ∼ 9 m. In order to achieve a competitive level of meson production, the H[−] beam is accelerated up to 500 MeV with a maximum beam loss of 6% [\[6\]](#page-15-1). This limits the peak B field to 0.576 T and thus, reduces the flutter at the

Figure 3: Integrated fractional dissociation of H[−] as a function of energy for different B.

highest energy. In order to compensate the effect of the reduced flutter, the spiral angle of the TRIUMF sectors is made so large especially at the higher energy region to ensure sufficient axial stability [\[7\]](#page-15-2).

3.3 H_2^+

 H_2^+ is a di-atomic ion with an equilibrium bond distance of about 1.06 Å. The binding energy of H_2^+ is about 2.7 eV, which is roughly 3 times larger than the binding energy of H[−]. Despite of a higher binding energy, some past experiments had shown evidence of Lorentz dissociation of H_2^+ at a much lower equivalent electric field $(\mathcal{E} < 1 \text{ MV/cm})$ [\[8,](#page-15-3) [9\]](#page-15-4). Due to the lack of experimental data at a higher field (typical range used in a cyclotron: $\mathcal{E} > 1$ MV/cm), some theoretical models have to be used as the preliminary tool to estimate the extent of Lorentz dissociation of H_2^+ .

In general, the presence of external Lorentz field tends to lower the asymptotic nuclear potential of the lower electronic state [\[10,](#page-15-5) Fig.3]. This increases the chance of H_2^+ at high-lying ν states to become unstable and a proton

"leak" from the molecular ion to disintegrate into a proton and a hydrogen atom. This is called the pre-dissociation of H_2^+ and it is the main dissociation mode of H_2^+ . Hiskes performed a series of calculations of the ionic lifetime of each vibrational state at different electric fields for H_2^+ at $J = 0$ [\[10\]](#page-15-5). Combining this information with the population of states determined by Busch et. al. [\[11\]](#page-15-6), we can estimate the maximum integrated fraction of dissociated beam at different $\mathcal E$ fields.

For instance, the equivalent electric field for a 100 MeV/u H_2^+ at 2 T is 2.8 MV/cm. At this \mathcal{E} , vibrational states up to $\nu = 15$ will dissociate in 10⁻⁸ s according to [\[10\]](#page-15-5). These unstable states amount to a total population of about 0.0035 [\[11\]](#page-15-6). This result is summarized in Fig. [4,](#page-9-0) of which similar case study at different B fields are also shown. A dissociation of about 0.35% of a 100 MeV/u H_2^+ corresponds to 200 W for a 0.28 mA beam. This is close to the practical limit from many experiences of other laboratories to allow a routine hands-on maintenance [\[12\]](#page-15-7). At higher energy, the equivalent electric field increases, and so does the Lorentz dissociation. For example, at energy of 500 MeV/u and B at 2 T, the total dissociated fraction is about 0.6%. Taking a maximum dissipated power of 200 W, the maximum allowed beam current is merely 33 μ A.

3.4 H_3^+

Ever since the first discovery of H_3^+ by J. J. Thomson in 1911, this simplest polyatomic molecule had gained immense research interest due to its high abundance in both laboratory-scale hydrogen discharges and the interstellar space [\[13,](#page-16-0) [14\]](#page-16-1). Its main structure of an equilateral triangle with an equilibrium distance of \sim 0.9 Å has provided a good symmetry and stability to the molec-ular ions [\[15,](#page-16-2) [16\]](#page-16-3). The binding energy (dissociation energy) of H_3^+ is about 4.5 eV, which is about 2 times larger than H_2^+ , and is thus the most stable among the hydrogen ions discussed in this work [\[17\]](#page-16-4). Despite its stability, any external field still has a tendency to lower the asymptotic potential of the molecular system, causing H_3^+ to pre-dissociate into a hydrogen molecule and a proton.

Owing to the complex dynamical structure of the non-linear tri-atomic

(b) Total dissociation of all state at B=1, 2, 3 and 5 T

Figure 4: A summary plot of the dissociated fraction of H_2^+ . (a) shows the contribution from individual unstable state when $B = 2$ T, while (b) shows the total dissociation from all ν states when B=1, 2, 3 and 5 T respectively. Each plateau (dashed line) in (a) indicates the maximum dissociated fraction at each ν state. This corresponds to the population of states in [\[11\]](#page-15-6). The blue curve is the summation of all vibrational states at B=2 T. As B increases from 1 to 5 T, the total dissociated fraction also increases up to \sim 2%.

molecule, only very few study were done so far to investigate directly the effect of external field on H_3^+ [\[18,](#page-16-5) [19,](#page-16-6) [20\]](#page-16-7). Reckzügel and the group is among the few who had looked into this for the case of a linear and triangular H_3^+ [\[19\]](#page-16-6). Fig. 5 in [\[19\]](#page-16-6) shows the change of the potential energy surface of a triangular H_3^+ as the external electric field increases. The higher electric field lowers the dissociation energy barrier, causing the ion to disintegrate more easily. The relationship between the dissociation energy (E_d) and $\mathcal E$ field (in MV/cm) extracted from [\[19\]](#page-16-6) is plotted in Fig. [6.](#page-11-0) The plot can be fitted by a quadratic function as follows:

$$
E_d = 4.5 - 0.025\mathcal{E} + 0.000036\mathcal{E}^2 \text{ (eV)}\tag{7}
$$

Figure 5: Fitted function of electric field and dissociation energy for triangularshaped H_3^+ using equation [7.](#page-10-0)

As a tri-atomic molecule, H_3^+ has two main vibrational modes: the symmetric "breathing" mode ν_1 , and the asymmetric "bending" mode, ν_2^l . In breathing mode, all the internuclear distances grow and shrink simultaneously. On the other hand, the bending mode is doubly degenerated and the molecule has a vibrational angular momentum l that is not divisible by 3. When $J = 0$, only the symmetry breathing mode exists. However, when $J > 0$, both modes exist. In fact, there are more than several hundreds of rotation-vibrational (ro-vibrational) states, including both ν_1 and ν_2 , that lie below the dissociation energy [\[21\]](#page-16-8). The full population of all these states with transition time is not an easy work. V. G. Anichich had computed a simpler estimation of the population of H_3^+ in only ν_1 states forming from [\[22\]](#page-17-0)

$$
H_2^+(\nu_i) + H_2(\nu_o) \to H_3^+(\nu_1) + H(1s)
$$
\n(8)

by using a cold H_2^+ beam (initial $\nu_o = \nu_i = 0$) [\[22\]](#page-17-0). The more detailed results of the population of excited states using different one- and two-anharmonic models can be found in [\[22\]](#page-17-0).

Using eqn. [7](#page-10-0) and the population of state of one-harmonic model from [\[22\]](#page-17-0), the integrated dissociated fraction of H_3^+ at different magnetic fields can be estimated. The results are shown in Fig. [6.](#page-11-0)

Figure 6: The maximum dissociated fraction from the population of unstable states of H_3^+ at B=2, 3 and 5 T respectively. This plot uses equation [7](#page-10-0) and the population of state from the one-harmonic model in [\[22\]](#page-17-0). Each plateau corresponds to a complete dissociation of all the particles at each ν_1 state.

Taking H_3^+ of energy 1 GeV/u under a constant B field of 3 T, the equivalent $\mathcal E$ is about 16.3 MV/cm. This corresponds to a dissociation energy of about 4.1 eV and a dissociation of less than 0.01% from Fig. [6.](#page-11-0) The result is similar even if the population of the more detailed two-anharmonic model from [\[22\]](#page-17-0) were used. If we assume a maximum beam loss of 200 W, beam energy up to 1 GeV/u is possible at a maximum beam current of 667 μ A at a radius of about 5.6 m. We can therefore infer that the effect of external Lorentz field onto the beam loss of H_3^+ is minimal at high-energy (> 500 MeV) extraction.

4 Comparisons of H ions

The particle's mass m_0 , radius ρ and magnetic field B are related to each other by

$$
B\rho = m_0 c \gamma \beta
$$

= $A \gamma \beta (3.1 \text{ Tm})$

Therefore, under the same energy per nucleon (same $\gamma\beta$), in order to keep the radius constant, a larger magnetic field is necessary to accelerate hydrogen ions with a higher molecular state. It is important to take into account of these physical factors in addition to the Lorentz dissociation when choosing the most suitable type of ion to achieve the desired beam power. Table [1](#page-13-0) summarizes important parameters to be considered when designing a cyclotron at three different energy regions for the three hydrogen ions discussed.

As for the calculation of maximum Lorentz dissociation in Table [1,](#page-13-0) a flutter component of $f_N = 0.5$ for $B = B_0(1+f_N \cos N\theta)$ and $N = 4$ was also included and the Lorentz loss was integrated over all turns up to the final energy using equation [5.](#page-6-0)

The comparison shows that the best candidate for acceleration up to 100 MeV/u is H[−]. This is due to its small effect of Lorentz dissociation and the highest cost efficiency with the least B field at the same extraction radius. However, as the beam energy increases, the significant Lorentz dissociation of H[−] outweighs this advantage. Thus, when the particle energy is more than 100 MeV/u, acceleration of H_2^+ or H_3^+ are the better options. The overall stability of H_3^+ is, however, slightly better than H_2^+ , despite the requirement of magnetic field is about 1.5 times higher. This is consistent with the study in [\[23\]](#page-17-1). At a very high energy up to 1 GeV, H_3^+ shall be the best option due

	$\rm H^-$	H_2^+	H_3^+
Energy (MeV/u)		100	
Momentum, $\beta\gamma$		0.47	
Extraction radius, ρ (m)		1.5	
Ave. B field, $B_0(T)$	1	$\overline{2}$	3
Peak B field (T)	1.5	3	4.5
Max. Lorentz dissociation $(\%)$	0.4	0.4	< 0.01
Energy (MeV/u)		500	
Momentum, $\beta\gamma$		1.2	
Extraction radius, ρ (m)		3.64	
Ave. B field, $B_0(T)$	1	$\overline{2}$	3
Peak B field (T)	1.5	3	4.5
Max. Lorentz dissociation $(\%)$	100	1	0.01
Energy (MeV/u)		1000	
Momentum, $\beta\gamma$		1.8	
Extraction radius, ρ (m)		5.65	
Ave. B field, $B_0(T)$	1	2	3
Peak B field (T)	1.5	3	4.5
Max. Lorentz dissociation $(\%)$	100	1.5	0.1

Table 1: Comparison of Lorentz dissociation of the three hydrogen ions discussed in this work. Note that the peak B field is obtained by assuming a flutter component of $f_N = 0.5$ for $B = B_0(1 + f_N \cos N\theta)$.

to its lowest Lorentz dissociation.

5 Conclusions and Prospects

This work compiled the estimation of Lorentz dissociation for three different types of hydrogen ions at different energy ranges. Overall, if physical factors such as a high magnetic field is allowed, H_3^+ is the best candidate for acceleration at energy greater than 100 MeV/u due to its lowest Lorentz loss and little interference at the center region after extraction. On the other hand, H[−] is the most cost efficient for low-energy acceleration up to $100 \text{ MeV}/u$. Stripping extraction of hydrogen ions is not suitable for beam power greater than 2 MW, as the power loss due to Lorentz dissociation is too prominent (> 200 W).

Nevertheless, the estimation given in this work, especially for H_2^+ and H_3^+ , are very approximate and many factors have been omitted. In fact, population at higher vibrational states with $J\neq 0$ exists and the total number of populated excited states may exceed the reported values from the literature used in this work. Besides, the effect of magnetic field and electric field on the accelerated field might not be entirely similar. In real practice, the Lorentz dissociation of H_2^+ is more complex and it could vary more than 10 times, as it highly depends on the initial beam condition $[9, 8]$ $[9, 8]$ $[9, 8]$. Some facilities have shown the feasibility to generate a high-intensity beam from an ion source for the production of hydrogen ions at different molecular states [\[24,](#page-17-2) [25\]](#page-17-3). Therefore, verification of Lorentz dissociation using real hydrogen ions from an ion source should be realistically feasible in the coming future. This shall be the most important work to be done before H_2^+ and H_3^+ ions can be fully implemented at a higher beam power.

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