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A Global Fitting Code for Multichordal Neutral Beam Spectroscopic Data

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Knowledge of the heat deposition profile is crucial to all transport analysis of beam heated discharges. The heat deposition profile can be inferred from the fast ion birth profile which, in turn, is directly related to the loss of neutral atoms from the beam. This loss can be measured spectroscopically by the decrease in amplitude of spectral emissions from the beam as it penetrates the plasma. The spectra are complicated by the motional Stark effect which produces a manifold of nine bright peaks for each of the three beam energy components. A code has been written to analyze this kind of data. In the first phase of this work, spectra from tokamak shots are fit with a Stark splitting and Doppler shift model that ties together the geometry of several spatial positions when they are fit simultaneously. In the second phase, a relative position-to-position intensity calibration will be applied to these results to obtain the spectral amplitudes from which beam atom loss can be estimated. This paper reports on the computer code for the first phase. Sample fits to real tokamak spectral data are shown.

INTRODUCTION

As a neutral heating beam penetrates a magnetically confined plasma, atoms are lost from the beam as they ionize and become trapped on magnetic surfaces. The initial spatial profile of these ions is referred to as the fast ion birth profile, and this profile is the source for any subsequent analysis of ion slowing down and neutral beam heat deposition. While the ions themselves cannot be detected directly, light emitted from the neutral beam atoms can be measured spectroscopically. By comparing the light emissions from two nearby points along such a beam one can infer that the difference in intensity must be due to the loss of those atoms that became ionized in the intervening space. Allowance must be made for viewing geometry, and the detector system must be calibrated in intensity to relate the signal amplitudes from the two spatial points to each another, but only a relative intensity calibration is required. On the DIII-D tokamak, the charge exchange recombination (CER) spectroscopy system can acquire beam emission spectra from multiple points that span the plasma from its edge all the way to the center.¹⁻³

To obtain the intensity of the beam emission spectra, one cannot simply add up the light intensity falling upon the individual wavelength channels. The spectral region may contain light from visible Bremsstrahlung, or from atoms or ions in the plasma that are not part of the neutral beam. There will also be contributions from detector dark current, dc offset in the amplifier, and other instrumental phenomena. For these reasons, the total spectrum must be fit with a theoretical model that can separate the beam emission spectra from all other effects.

The model must contain as much physics as possible in order to fit the data as precisely as possible and also to minimize the number of free parameters. Two of these pieces of physics are the Doppler effect, which shifts the lines emitted by the fast-moving beam atoms, and the motional Stark effect, which causes each line to be split into a manifold of 15 related peaks. The motional Stark effect is caused by the intense electric field the beam atoms experience in their rest frame as they cross the tokamak's magnetic field at high speed.

The ultimate goal of this analysis is to determine neutral beam atom density as a function of position in the plasma. When this beam penetration analysis becomes routine, it will be useful both for beam deposition profile analysis and for helium

transport studies.⁴ Knowledge of helium transport rates is absolutely critical for the design of future fusion reactors.

The present paper discusses the status of the computer code used to fit the model to the spectral data and shows examples of the results.

I. PHYSICS OF THE NEUTRAL BEAM SPECTRA

The system used to gather the data is a set of visible spectrometers known as the Charge Exchange Recombination (CER) spectroscopy system. Its features and capabilities are described in the references.¹⁻³ By tuning the spectrometers a few tens of Å away from the H α line ($n = 3 \rightarrow 2$, $\lambda_0 = 6562.8\text{Å}$), Doppler shifted emissions from the fast moving beam atoms can be seen. At the edge of the plasma these spectra are strong and distinct (Fig. 1), but, as more and more beam particles are lost via ionization, the neutral signal from deeper inside the plasma becomes weak and noisy (Fig. 2). All the spectra are complicated by two things: multiple beam species and the motional Stark effect. To correctly fit these data, the code incorporates both of these effects into its model.

For hydrogen or deuterium, positive ion beam sources produce three beam energy species: one at the full energy of the beam acceleration voltage, and one each at one-half and at one-third of this energy. Each species undergoes collisional excitation with plasma ions and electrons to produce its own spectral peak, and the peak wavelengths are related to one another by the Doppler shift physics which depends upon the velocity of the beam atoms, v , and the angle between the beam and the direction of view, θ . Since there is also hydrogen or deuterium in the surrounding plasma, light from λ_0 will also appear, and its wavelength will be related to the beam peaks by the same Doppler shift.

Fast beam neutrals moving across the strong magnetic field in the tokamak experience an electric field in their rest frame. This field is given by the Lorentz relation Eq. (1)

$$\vec{E} = \vec{v} \times \vec{B} = v B \sin \phi \quad , \quad (1)$$

where v is the beam velocity, B is the local magnetic field and ϕ is the angle between them. This field gives rise to a Stark splitting of each beam peak into a manifold of

Fig. 1. A good quality neutral beam emission spectrum from the edge of the plasma. The vertical axis is intensity in arbitrary units, and the horizontal axis is wavelength in units of detector pixels with blue to the left. The tiny crosses are the raw data points, and the solid curve is the theory line for this fit. The Stark manifolds for the full, half, and third energy beam components are labeled. Before fitting, the contrast was enhanced slightly by subtracting the signal from a time 100 msec earlier when the neutral beams were off. These data are from a 75 keV hydrogen beam injected into a 2.1 Tesla (on-axis) hydrogen plasma. The small plot below is the residuals for the fit.

15 lines, all of which have exactly the same width ("temperature") and whose spacing is proportional to the strength of the electric field. Only nine of these lines have appreciable intensity, and they are grouped into two polarizations called π (linearly polarized parallel to E) and σ (linearly polarized perpendicular to E). The amplitudes of these lines depend upon the transition strength, the population of the upper level, and the direction of view with respect to the electric field.

Fig. 2. Poorer quality data from the center of the plasma. This is the same shot and time as for Fig. 1. Fewer beam particles produce a much weaker signal. The larger beam-chord angle here produces a smaller Doppler shift which causes the full, half, and third energy beam peaks to crowd closer together. The Stark splitting is only slightly larger, though, because the path of the beam is such that $\vec{v} \times \vec{B}$ is a weak function of major radius. Again, timeslice subtraction was used to enhance contrast.

II. NEUTRAL BEAM SPECTRAL ANALYSIS

The code to fit these neutral beam emission spectra is a χ^2 minimizing non-linear least-squares fitter and has been dubbed STARKERS. It fits multiple spectral peaks to each spectrum and can fit multiple spectra from different spatial positions simultaneously (up to eight positions, maximum). The unit of analysis is the theoretical Gaussian lineshape convolved with the spectrometer's instrumental response. The instrumental response is defined to be the normalized output of the linear photodiode detector¹⁻³ when a single arbitrarily narrow spectral line is presented at the spectrometer's entrance slit. We have found from experience that the instrumental

response is well approximated by a sum of two or three Gaussians.¹ For the simplest case, that of an impurity line with completely free amplitude, location and width, the fitting function is given by Eq. (2)

$$I_i(A_{j,k}, w_{T,j,k}, \text{LOC}_{j,k}) = A_{j,k} \sum_{n=1}^{n_{\text{gauss}}} \frac{\alpha_n w_n}{(w_{T,j,k}^2 + w_n^2)^{1/2}} \exp \left[-\frac{(i - \text{LOC}_{j,k} + sh_n)^2}{(w_{T,j,k}^2 + w_n^2)} \right] \quad (2)$$

On the left hand side of Eq. (2) I_i is the signal amplitude at the detector's i^{th} pixel, and on the right hand side is the contribution to this signal from the j^{th} spectral peak of the k^{th} spatial position. $A_{j,k}$ is its peak amplitude, $\text{LOC}_{j,k}$ is its location (in units of pixels), and $w_{T,j,k}$ is its width (also in pixels). Parameters with the subscript n are associated with the instrumental response with α_n being the amplitude, w_n the width, and sh_n a small relative wavelength displacement between the member Gaussians of the instrumental response (usually the instrumental response is symmetric and so all the sh_n are zero). The sum over n totals the contributions of these individual Gaussians.

For the next more complicated case of beam-into-gas with no magnetic field, the beam peak locations are related to each other by the Doppler shift, but there is no Stark splitting because the field is zero. This situation is modeled by Eq. (3),

$$I_i(A, w_T, \text{LOC}) = \sum_{j=1}^{n_{\text{peaks}_k}} A_{j,k} \sum_{n=1}^{n_{\text{gauss}}} \frac{\alpha_n w_n}{(w_{T,j,k}^2 + w_n^2)^{1/2}} \exp \left[-\frac{(i - \text{LOC}_{j,k} + sh_n)^2}{(w_{T,j,k}^2 + w_n^2)} \right] \quad (3)$$

where the sum over j includes the full, half, and third energy beam peaks plus the thermal H_α peak at λ_0 . Not all of these have to be included in a fit, but there must be at least two for the Doppler shift calculation. Again $\text{LOC}_{j,k}$ is the center of the j^{th} peak. For one of the j s, $\text{LOC}_{j,k}$ will be a free fit parameter, and for all other values of j $\text{LOC}_{j,k}$ will be calculated by the Doppler shift physics from v and θ . While θ is

different at each spatial position, v is the same for all positions and is thus a global fit parameter. For improved accuracy, the Doppler shift model used is a relativistic one, and it has been expanded out to terms in $(v/c)^4$ in order to avoid subtracting two numbers of comparable magnitude.

Figure 3 shows such a beam-into-gas spectrum. The full, half, and third energy beam peaks were fit with the model of Eq. (3), and the two spectral features at pixel 116 (between the half and third energy beam peaks) and pixel 192 (far right) were fit with the model of Eq. (2). The peak at 192 is an impurity line. The peak at 116 is used to model the neutral beam stragglers which result from ions in the neutral beam injector that neutralize before they receive the full effect of the acceleration voltage.⁵ While this single-Gaussian “model” for the stragglers is not based on any physics, including them in this way results in a much better fit for other nearby peaks and in this instance reduced χ^2 by a factor of four.

Finally, the Stark splitting model is given by Eq. (4).

$$I_i(A, w_T, LOC) = \sum_{j=1}^{n_{\text{peaks}_k}} A_{j,k} \sum_{\pi, \sigma}^{3 \text{ or } 6} a_{\pi, \sigma} \sum_{n=1}^{n_{\text{gauss}}} \frac{\alpha_n w_n}{(w_{T,j,k}^2 + w_n^2)^{1/2}} \exp \left[-\frac{(i - LOC_{j,k} + sh_n + N_{\pi, \sigma} \Delta \lambda_j)^2}{(w_{T,j,k}^2 + w_n^2)} \right], \quad (4)$$

Here $LOC_{j,k}$ is the center of each Stark manifold and the individual peaks are centered at $N_{\pi, \sigma} \Delta \lambda$. The $N_{\pi, \sigma}$ are small integers that range from -4 to $+4$ selecting the individual Stark peaks, and $\Delta \lambda$ is a constant times the electric field of Eq. (1) divided by the spectral dispersion to convert Å into pixels. The $a_{\pi, \sigma}$ s are the relative amplitudes of each π or σ manifold member, and their values are fixed by the assumption of statistical population of the atomic levels.

Since the optics of the CER diagnostic were not designed to preserve polarization, we make no claim about the relative amplitude between the π and σ members of a Stark manifold, and these amplitudes are allowed to be free with respect to one

Fig. 3. Fit spectrum of hydrogen beam-into-gas with no magnetic field. In addition to the raw data and theory line, each spectral feature is shown individually as a dotted Gaussian.

another. This is done by having two $A_{j,k}$ s for each manifold, one for the π peaks and one for the σ peaks.

In summary, for each Stark manifold there are four principal parameters: one width, one amplitude for the π peaks, one amplitude for the σ peaks, a location for the center of the manifold (which may be a free parameter itself or depend upon v and θ), and a wavelength splitting (which depends upon v , B and ϕ). At this writing, there is insufficient geometry in the model to fit B separately from ϕ , and so the product $B \sin \phi$ is treated as one parameter. Thus, a manifold of nine close-lying Gaussian peaks is fit with only six free parameters. The Stark manifolds of all three beam components (full, half, and third) from a single spatial position are also related to each other since B , ϕ and θ are the same for all, and the particle velocities are ratioed $1 : 1/\sqrt{2} : 1/\sqrt{3}$ which further reduces the number of free parameters.

In addition to these spectral models, the background can be modeled as having either a constant, linear, or quadratic form.

III. CURRENT STATUS OF WORK

The STARKERS code is written to fit data from 2000 pixels (250 each from a maximum of eight spatial positions) with 257 free parameters in a single fit. Test fits of ~ 1100 points and ~ 100 free parameters have been done. The code also has a flexible user interface to enter commands and display information.

Figures 1 and 2 show examples of a Stark splitting fit from a plasma shot. In addition to the raw data and the theory line, each Stark peak is marked by a vertical bar whose height is proportional to the peak's amplitude and whose top is capped by a π or a σ indicating the polarization. At large major radius (Fig. 1), the Stark peaks for the half and third energy beam components are just separated. At small major radius (Fig. 2), they overlap extensively. Also notice the difference between the relative amplitudes of the full, half, and third energy beam components for these two spectra. The lower energy fractions have poorer penetration and so are greatly attenuated deep inside the plasma (Fig. 2). In the fit for Fig. 1, a single broad peak was used to model the beam stragglers, and it is shown by a T-topped marker near pixel number 129. The fit for Fig. 2 did not require this feature.

Figure 4 shows a fit for a deuterium beam-into-gas shot at 0.9 Tesla. The slower moving deuterium and the lower B-field combine to produce a much smaller Stark splitting. This is for the same spatial position as the fit in Fig. 1.

The quality of the fits for the spectra shown is excellent. The theory lines go through all the data points, and the residuals are small and random in nature. While fits to spectra like Figs. 1 and 4 might be attempted with a general Gaussian fitting code (*i.e.*, a code in which each peak has completely free width, amplitude, and location) by approximating sets or subsets of adjacent Stark peaks with single, broader Gaussians, it would not work well at small signal-to-noise or at values of the Stark splitting intermediate between that in Figs. 1 and 4. This approximation technique would fail completely for spectra like that of Fig. 2. Only the detailed Doppler shift and motional Stark effect physics model can succeed in all of these

Fig. 4. Shown are the raw data, theory line, and Stark peak markers for a deuterium beam-into-gas shot at $B = 0.9$ Tesla. Compare this with the spectrum in Fig. 1. The slower moving deuterium atoms and lower magnetic field combine to produce much smaller Stark splitting. A single broad peak has been inserted between the half and third energy peaks to account for the beam stragglers.

cases. Having built the tool that we need to analyze Stark-split spectra, we can proceed to determine beam densities and study beam deposition.

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