Non-linear Fitting of Charge Exchange Recombination Spectra with Energy-Dependent Cross Section Included

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2002 APS-DPP Meeting

Nov 11-15, 2002
Orlando, Florida
Overview of Poster

♦ Poster is about measurements of $T_i$ and $V_{tor}$ via Charge Exchange Recombination (CER) Spectroscopy

♦ Details of the CER cross section affect the observed spectra
  - Apparent shifts in $T_i$ and $V_{tor}$ can be obtained if the “cross section effect” is ignored

♦ This poster documents the development of algorithms for fitting of the observed spectra with cross section effect included

♦ Cross section is modeled in non-linear least squares analysis of data, rather than via post-processing
The problem: spectrum produced by charge exchange recombination of a thermal population of plasma ions with the fast neutrals of a neutral beam

\[ \text{E.g. } D^0 + C^{6+} \rightarrow D^+ + (C^{5+})^* \rightarrow D^+ + C^{5+} + \text{photon} \]

To lowest order, the spectrum is a shifted Gaussian in wavelength space.

However, cross section for CER process varies as a function of relative velocity between ions and beam atoms.

- Spectrum is modified - lowest order analysis will have systematic offsets of temperature and rotation velocity.
Geometry for Horizontal View

- $\delta$ is angle between view chord and neutral beam
- In DIII-D, typical $\delta$ for core views is 40-45°
Effective Emission Rates

“Cross Section Effect” for $T_i$ for CVI 5290

Apparent Ti from Gaussian Fit to CXRS Spectrum
C VI 5290.5A, $E(D^0) = 40$ keV/amu

$T_{true} - T_{app}$ (keV)

$T_{true}$ (keV)

$\delta = 50^\circ$

$\delta = 30^\circ$

$\delta = 10^\circ$
“Cross Section Effect” for $V_{tor}$ for CVI 5290

Apparent Velocity from Gaussian Fit to CXRS Spectrum
C VI 5290.5A, $E(D^0) = 40$ keV/amu

\[ V_{true} - V_{app} \text{ (km/s)} \]

\[ T_{true} \text{ (keV)} \]

\[ \delta = 50^\circ \]
\[ \delta = 30^\circ \]
\[ \delta = 10^\circ \]
Post-processing Is Often Used to Account for the “Cross Section Effect”

♦ Cross section effect is well known and studied

♦ Typically, this effect produces a spectrum which is very close to Gaussian in shape
  o Spectrum exhibits apparent shifts of rotation and temperature relative to true parameters for emitting ions

♦ Post-processing often used to correct cross section effect
  o Fit Gaussian to experimental spectrum with least squares and then correct for apparent Ti and rotation shifts
“Cross Section Effect” Can Be Accommodated Directly in Least Squares Fitting of Data

♦ Post-processing has potential drawback
  o If cross section effect produces spectrum which is not sufficiently Gaussian, post-processing may introduce error

♦ Fitting to a model with cross section effect included avoids this problem
  o The price is a more complicated and slower analysis procedure because the fitting model cannot be specified in a completely analytic form

♦ This poster documents the development of algorithms for the direct fitting of the spectrum with cross section effect included
Fit Model Based on Velocity Integrals Which Include CER Cross Section

Following von Hellermann, the spectrum line-shape is:

\[ f(v_z) = \frac{1}{\pi^{3/2} v_{th}^3} \int d^3 \vec{v} Q(\|\vec{v} - \vec{v}_b\|) \delta(v_z' - v_z) \exp \left[ -\left( \frac{\vec{v} - \vec{V}}{v_{th}} \right)^2 / v_{th}^2 \right] \]

Where:

- line of sight is along z-axis
- \( \vec{v}_b \) is the velocity of the beam neutrals
- \( \vec{V} \) is the flow velocity of the emitting ions
- \( v_{th} \) is the thermal velocity of the ions
- \( Q(\|\vec{v}\|) = \sigma_{cx}(\|\vec{v}\|)\vec{v} \) is the effective excitation rate for a charge exchange event with cross section \( \sigma_{cx} \)

Use von Hellermann’s analytic expression for \( Q \)
Evaluation of Velocity Space Integral Has been Performed in Three Ways

- Evaluation over $v_z'$ is trivial due to delta function
- The remaining integral is a 2D integral over $v_x'$ and $v_y'$
- Burrell has exploited a symmetry in the problem to turn the 2D integral into an exact 1D integral
- Burrell has also obtained an approximate analytic solution for the 1D integral
- Thus, integral can be evaluated via
  - 1) Numerical evaluation of exact 2D form
  - 2) Numerical evaluation of exact 1D form
  - 3) Analytic evaluation of approximation 1D form
The Three Forms for Velocity Space Integrals Have Been Successfully Implemented

- Testing shows that numerical evaluation of the 2D and 1D forms of the exact integrals agree, as expected.
- For C VI 5290, the evaluation of the 1D analytic form of the integral agrees well with the numerical evaluation for $T_i$ up to 15-20 keV.
- Evaluation of the 1D analytic form is 2 orders of magnitude faster than numerical evaluation of the exact 2D form.
1D Analytic Function for C VI 5290 Is Good Approximation to 2D form for $T_i$

Apparent $T_i$ from Fit of Analytic Approx to CXRS Spectrum
C VI 5290.5A, $E(D^0) = 40$ keV/amu

![Graph showing differences between 2D and analytic functions for $T_i$ at different angles $\delta$.]
1D Analytic Function for C VI 5290 Is Good Approximation to 2D form for $V_{\text{tor}}$

Apparent Velocity from Flt of Analytic Approx to CXRS Spec
C VI 5290.5A, $E(D^0) = 40$ keV/amu

$V_{2D} - V_{\text{analytic}}$ (km/s)

$T_{2D}$ (keV)

$\delta = 10^\circ$

$\delta = 30^\circ$

$\delta = 50^\circ$
Implementation of Model for CER Spectrum in Least Squares Fitting

♦ The 1D numerical and analytic forms of the velocity integral have been incorporated into least squares fitting of experimental data

♦ Implemented in CERFIT, code used to fit experimental DIII-D CER spectra
  o To obtain ion temperature, rotation velocity and amplitude

♦ CERFIT is a fortran-90 code

♦ Modular programming used to implement the model for CER spectrum

♦ Algorithms developed to maximize speed while retaining required accuracy
Mechanics of Non-Linear Fitting

Perform initial fit using Gaussian model

Estimate cross section effect on $T_i$ and $V_{tor}$

Perform non-linear least-squares minimization
  Fit to model which is sum of CER peak plus Gaussians
  Perform numerical convolution of instrumental function with model spectrum
  Compute chi-squared

Compute error bars
Perform initial fit using Gaussian model

- Problem initialized with standard Gaussian fit to experimental spectrum
- This model treats the spectrum as sum of Gaussians
  - Includes the CER line
  - May include a passive edge line from same ion
  - May include other edge lines
Estimate Cross Section Effect on $T_i$ and $V_{tor}$

- Gaussian model produces good fit to CER spectrum
- However, the $T_i$ and $V_{tor}$ which are produced by the fit will have apparent shifts
- These apparent shifts are estimated from the 1D analytic model for the spectrum
- The $T_i$ and $V_{tor}$ parameters are corrected for apparent shifts and used as initial guesses for the next step of the fit
- Amplitude parameter from Gaussian fit is passed through to the next step
Perform Least-squares Minimization with CER Model

- Fit to a model in which CER line is modeled with CER spectrum and other lines are treated as Gaussians
  - In fact, CER line is sum of 3 (6) CER spectra due to 3 energy components of 1 (2) neutral beams
  - Ratios of energy components obtained from beam attenuation calculations which are available from a database
- Instrumental function is convoluted numerically with model spectrum
  - Convolution performed with QUADPACK routine DQNG, a non-adaptive definite integral routine
  - Speed-up (~100X) obtained by evaluating model spectrum once and fitting with spline for use in the convolution
Perform Least-squares Minimization - continued

- Non-linear minimization is performed with *SLATEC* routine *DNLS1E*
  - A Levenberg-Marquardt routine
  - Performs numerical derivatives of chi-squared with respect to the fit parameters
- After fit is completed, error bars are computed from covariance matrix
  - Covariance matrix obtained with *SLATEC* routine *DCOV*
  - *DCOV* numerically obtains the Jacobian, required for the covariance matrix
Model with Cross Section Effect Brings He II and C VI Temperatures into Agreement

Fit with Gaussian
Fit with CER Cross Section

![Graphs showing temperature profiles](image-url)
Model with Cross Section Effect Increases Rotation Velocities Substantially

Fit with Gaussian

Fit with CER Cross Section

LEGEND
■ = C VI 5290
● = He II 4686
Initial Conclusions

♦ For ion temperature, use of CER cross section vs pure Gaussian model (for DIII-D geometry) →
  o Small increases of $T_i$ for C VI
  o Moderate increases $T_i$ for He II
  o Tends to bring $T_i$ for He II and C VI into agreement

♦ For toroidal rotation, use of CER cross section vs pure Gaussian model (for DIII-D geometry) →
  o Moderate increases of $V_{tor}$ for C VI and for C VI
  o Does not bring $V_{tor}$ for He II and C VI into full agreement
    – This result is potentially a neoclassical effect
    – See Baylor, RP1.030, this session
Status

♦ Software and testing have been completed for direct least squares fitting of CER spectrum with a model which includes the CER cross section effect
  o For horizontal views
♦ Benchmarking of results against post-processing technique has not yet been performed