§1. Atomic Data Evaluation and Data Fitting

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Charge transfer process between impurity ions and neutral hydrogen from neutral beam injection (NBI) or hydrogen atoms in peripheral region is one of important atomic processes in fusion plasmas and provides information on impurity ions, plasma transportation, physical conditions etc. as emission lines for plasma diagnostics. In order to obtain better results from data analysis of plasma diagnostics measurements, we need reliable atomic data for such atomic processes. Data evaluation is important to provide better atomic data. At the same time data fitting with analytic formulae is also important to provide evaluated atomic data in forms which are easily handled for analyses or simulations.

We have worked on making a computer program for data fiting with nonlinear analytic functions in order to proceed to data evaluation and fitting. Usually fitting function for cross sections of charge transfer processes and other collisional processes such as collisional excitation and ionization is assumed a nonlinear function empirically with asymptotic behavior at high energy.

For data fitting the method of least squares is commonly used: a parameter p of model function $f(x:p)$ needs to be obtained as minimizing a sum $F(p) = 0.5\sum_i[y_i - f(x_i : p)]^2$. Here we use the Levenberg-Marquardt method [1] which is the standard method for nonlinear least-squares routines for making the fitting program. This solves following equations for the Jacobian matrix $J(p) \doteq \{\partial f(x_i : p)/\partial p_j\}$ with adusting a factor $\lambda^{(k)}$ for convergence:

$$[J(p^{(k)})^T J(p^{(k)}) + \lambda^{(k)} D^{(k)}]\Delta p^{(k)} = -J(p^{(k)})^T\{f(x : p^{(k)} - y\} \quad (1)$$

where $D^{(k)}$ is a diagonal matrix such as the unit matrix I.

Using the program, we fitted the experimental data of the charge exchange cross sections of Li ions and H atoms [3, 4] as shown in Figs. 1 and 2. We use the fitting function from Janev et al.(1993) [2],

$$\sigma(E) = \frac{a_1 \exp[-(a_2/E)^{a_3}]}{1 + (E/a_4)^{a_5} + (E/a_6)^{a_7} + (E/a_8)^{a_9}} \quad (2)$$

where $a_1 - a_9$ are fitting parameters, and obtained good fitting results with this program.

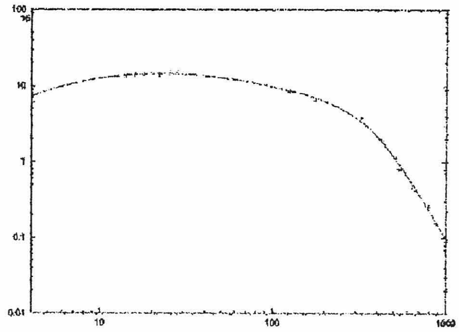

Fig. 1: Cross section for charge transfer process $Li^{2+} + H \rightarrow Li^+ + H^+$ [3,4]. X and Y axes are normalized with arbital units. Solid line is the fitted function.

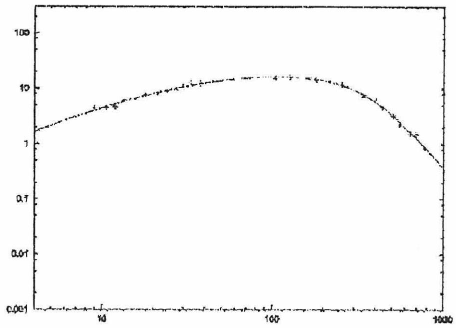

Fig. 2: Cross section for charge transfer process $Li^{3+} + H \rightarrow Li^{2+} + H^+$ [3,4]. X and Y axes are normalized with arbital units. Solid line is the fitted function.

References

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