A Method for Ion Distribution Function Evaluation Using Escaping Neutral Atom Kinetic Energy Samples

P.R. Goncharov, T. Ozaki, E.A. Veshchev, S. Sudo

National Institute for Fusion Science, 322-6 Oroshi-cho, Toki, 509-5292, Japan

A reliable method to evaluate the probability density function for escaping atom kinetic energies is required for the analysis of neutral particle diagnostic data used to study the fast ion distribution function in fusion plasmas. Digital processing of solid state detector signals is proposed in this paper as an improvement of the simple histogram approach. Probability density function for kinetic energies of neutral particles escaping from the plasma has been derived in a general form taking into account the plasma ion energy distribution, electron capture and loss rates, superposition along the diagnostic sight line and the magnetic surface geometry. A pseudorandom number generator has been realized that enables a sample of escaping neutral particle energies to be simulated for given plasma parameters and experimental conditions. Empirical probability density estimation code has been developed and tested to reconstruct the probability density function from simulated samples assuming Maxwellian and classical slowing down plasma ion energy distribution shapes for different temperatures and different slowing down times. The application of the developed probability density estimation code to the analysis of experimental data obtained by the novel Angular-Resolved Multi-Sightline Neutral Particle Analyzer has been studied to obtain the suprathermal particle distributions. The optimum bandwidth parameter selection algorithm has also been realized.

Keywords: neutral particle analysis, ion distribution, statistical data processing, empirical probability density, kernel bandwidth selection

1. Introduction

Measurements of kinetic energy distributions of neutral atoms escaping from magnetically confined plasma are used in controlled fusion experiments as a method to investigate the ion component distribution function and its evolution due to the application of various plasma heating schemes. The ion distribution function reflects the kinetic effects, the single particle confinement properties depending on the particular magnetic configuration, the finite β effects such as MHD induced fast ion losses, radial electric field effects, etc. The nuclear fusion reaction rate is determined by the ion distribution and thus its studies at suprathermal energies near the rate coefficient curve maximum are of primary importance. Advanced neutral particle diagnostics based on solid state detectors with high energy resolution, e.g. [1], are used to study the suprathermal ion distribution function. Statistical data processing is required to obtain a smooth normalized probability density function for particle energies using the measured random samples [2].

2. Escaping Neutral Particle Energy Distribution

The probability density function (PDF) *f(E)* for kinetic energies of neutral H^0 particles escaping from the plasma of a magnetic confinement fusion device in a general form is given by

$$f(E) = A e^{\int_{\rho_{\min}}^{1} Q^{-}(\tilde{\rho})\lambda_{mfp}^{-1}(E,\tilde{\rho})d\tilde{\rho}} \int_{\rho_{\min}}^{1} g(E,\rho) \times \left[Q^{+}(\rho) e^{-\int_{\rho_{\min}}^{\rho} Q^{+}(\tilde{\rho})\lambda_{mfp}^{-1}(E,\tilde{\rho})d\tilde{\rho}} - Q^{-}(\rho) e^{-\int_{\rho_{\min}}^{\rho} Q^{-}(\tilde{\rho})\lambda_{mfp}^{-1}(E,\tilde{\rho})d\tilde{\rho}} \right] d\rho \qquad (1)$$

where A is the normalization constant. The source function for H^0 atoms of energy E within the plasma

$$g(E,\rho) = n_i(\rho) f_i(E,\rho) \sum_l n^{(l)}(\rho) \langle \sigma \mathrm{v} \rangle^{(l)} \qquad (2)$$

is expressed via the local plasma proton distribution $n_i(\rho) f_i(E,\rho)$ and the sum of rates over all targets for the electron capture process. The derivatives $Q^{+}(\rho) = d\Lambda/d\rho > 0$ and $Q^{-}(\rho) = d\Lambda/d\rho < 0$ of the sight line distance Λ along the two intervals between $\rho = 1$ and $\rho = \rho_{\min}$ are obtained from the known structure of magnetic surfaces $\rho = const$. The neutral flux attenuation enters in the form of Poisson exponents, where $\lambda_{mfp}(E, \rho)$ is the H^0 mean free path with respect to all electron loss reactions.

author's e-mail: pavel@nifs.ac.jp

3. Numerical Experiment

Ideally, the passive diagnostic data is an array (E_1, …, E_N) of energies of escaped neutral particles measured along a certain observation direction, and N is the total number of particles collected during a certain time interval. This array is a sample of realizations of the random variable E distributed according to the law (1). Such form of data is achievable with solid state detectors by using pulse height analysis techniques, while the other analyzers, e.g. $\vec{E} \parallel \vec{B}$ ones, intrinsically form a histogram of the incoming particle energies over a certain number of subintervals called energy channels. Technical details may be found in [1]. The formulation of the problem considered here is to obtain an estimate $f^{*)}(E)$ of the unknown exact probability density function $f(E)$ of neutral particle energies from the experimental data. The sought function preferably should satisfy a specified precision criterion. The obtained PDF estimate is then to be used to reconstruct the ion distribution for further analysis.

Assuming a predefined theoretical PDF $f(E)$ one can carry out a numerical experiment by generating a sample of escaped atom energies for given plasma parameters and experimental conditions. We apply the inverse cumulative distribution function (CDF) approach. First, a sample of pseudorandom numbers (u_1, …, u_N) uniformly distributed within the $[0,1)$ interval is generated using an algorithm from [3]. Then, the energy values are calculated as solutions of the equation

$$F(E_j) = u_j, \tag{3}$$

where $$F(E) = \int_0^E f(\tilde{E})d\tilde{E} \tag{4}$$

is the CDF. These simulation results can be supplied as input data for the PDF estimation procedure to test its performance, since the original exact $f(E)$ used in the simulation is known.

Two typical ion energy distribution laws have been used in the numerical simulation, namely, (a) Maxwellian distribution with ion temperature T_i

$$f_i(E) = \frac{2}{\sqrt{\pi}} \frac{1}{T_i} \sqrt{\frac{E}{T_i}} \exp(-E/T_i), \tag{5}$$

$$F_i(E) = \frac{2}{\sqrt{\pi}} \gamma\left(\frac{3}{2}, \frac{E}{T_i}\right), \tag{6}$$

where $\gamma(\alpha, x) = \int_0^x t^{\alpha-1} e^{-t} dt$ is the lower incomplete gamma-function; and (b) the classical slowing down distribution for a delta-like fast ion source function

$$S(v - v_0) = \frac{S_0}{4\pi v^2} \frac{e^{-\frac{(v-v_0)^2}{\epsilon^2}}}{\epsilon\sqrt{\pi}} \tag{7}$$

$$f_i(v) = \frac{S_0}{8\pi} \frac{\tau_s}{v^3 + v_c^3} \left(erf\left(\frac{v^*(v,t) - v_0}{\epsilon} \right) - erf\left(\frac{v - v_0}{\epsilon} \right) \right) \tag{8}$$

where the slowing down time $\tau_s = \frac{3 m_p T_e^{3/2}}{4\sqrt{2\pi} n_e e^4 \Lambda m_e^{1/2}}$, the critical velocity $v_c^3 = \frac{3\sqrt{2\pi} T_e^{3/2}}{2 m_p m_e^{1/2}}$, Λ is the Coulomb logarithm, and $v^*(v,t) = \left((v^3 + v_c^3) e^{3t/\tau_s} - v_c^3 \right)^{1/3}$ [4]. The ion velocity $v = \sqrt{2E/m_p}$, v_0 is the injection velocity, S_0 and ϵ determine the source rate and width, and t is the time. Fig. 1 (a) shows the Maxwellian PDF for two different T_i values and Fig 1 (b) shows the classical slowing down PDF at t = 0.8 s for injection energy E_0 = 150 keV and two different pairs of the target plasma n_e and T_e values. Histograms of the corresponding pseudorandom number samples governed by these PDFs are shown in Fig. 1 (c) and (d).

4. Data Processing Method

As an improvement of the neutral particle diagnostic data analysis, we have applied the probability density estimation using kernel smoothing techniques, e.g., [5, 6]. The kernel PDF estimate

$$f^{(K)}(E) = \frac{1}{Nh} \sum_{j=1}^{N} K\left(\frac{E - E_j}{h} \right), \quad h > 0 \tag{9}$$

is determined by the kernel function $K(z)$ and the kernel bandwidth h. The performance criterion of this method is the value of the mean integrated squared error

$$MISE(f^{(K)}, f) = \left\langle \int_0^{+\infty} \left[f^{(K)}(E) - f(E) \right]^2 dE \right\rangle, \tag{10}$$

where averaging is over different samples of N realizations (E_1, …, E_N), and its "asymptote" for $N >> 1$ (large sample approximation)

$$AMISE(f^{(k)}, f) = \frac{c_1}{Nh} + \frac{c_2 c_3^2 h^4}{4}, \tag{11}$$

where $c_1 = \int K^2(z)dz$, $c_2 = \int (f''(z))^2 dz$ and $c_3 = \int z^2 K(z)dz$. The optimum kernel derived in [7] is $K(z) = \frac{3}{4}(1 - z^2) I_{(-1,\,1)}(z)$, where $I_{(-1,\,1)}(z)$ equals unity within (-1, 1) and equals nought outside. However, it is emphasized [5, 6] that the choice of the kernel function shape has a small influence on the method performance, while the bandwidth parameter choice is more important. Therefore, Gaussian kernel

$$K(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2} \tag{12}$$

has been used, since it has continuous derivative.

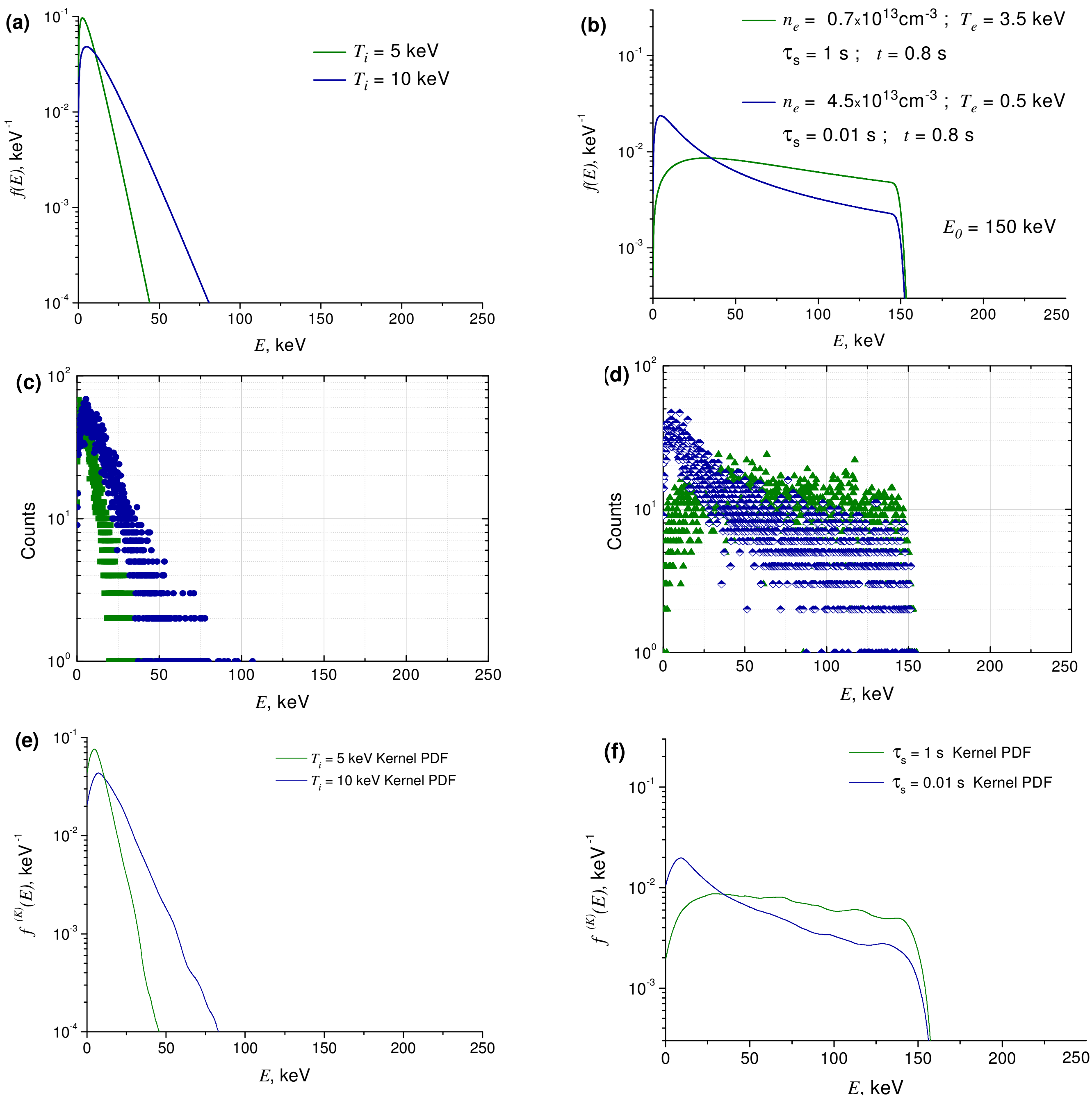

Fig. 1. (a) Maxwellian PDF for $T_i = 5$ keV (green) and $T_i = 10$ keV (blue); (b) classical slowing down PDF for τ_s = 1 s (green) and τ_s = 0.01 s (blue); (c) histograms of pseudorandom number samples distributed according to the laws shown in (a); (d) histograms of pseudorandom number samples distributed according to the laws shown in (b); (e) kernel PDFs calculated from Maxwellian law pseudorandom number samples shown in (c); (f) kernel PDFs calculated from slowing down distribution law pseudorandom number samples shown in (d).

A reliable practical method for optimum h selection was proposed in [8] and revisited recently in [9]. The bandwidth is sought by solving the equation

$$h = \left(\frac{1}{2\sqrt{\pi} N \phi_4(\eta(h))} \right)^{1/5}, \tag{13}$$

where the function ϕ_r is expressed via kernel derivative

$$K^{(r)}(z) = (-1)^r He_r(z) K(z) \tag{14}$$

as follows

$$\phi_r(h) = \frac{1}{N(N-1)h^{(r+1)}} \sum_{i=1}^{N} \sum_{j=1}^{N} K^{(r)} \left(\frac{E_i - E_j}{h} \right). \tag{15}$$

The function

$$\eta(h) = \left(\frac{-6\sqrt{2}\phi_4(a)}{\phi_6(b)} \right)^{1/7} h^{5/7} \tag{16}$$

depends on the values

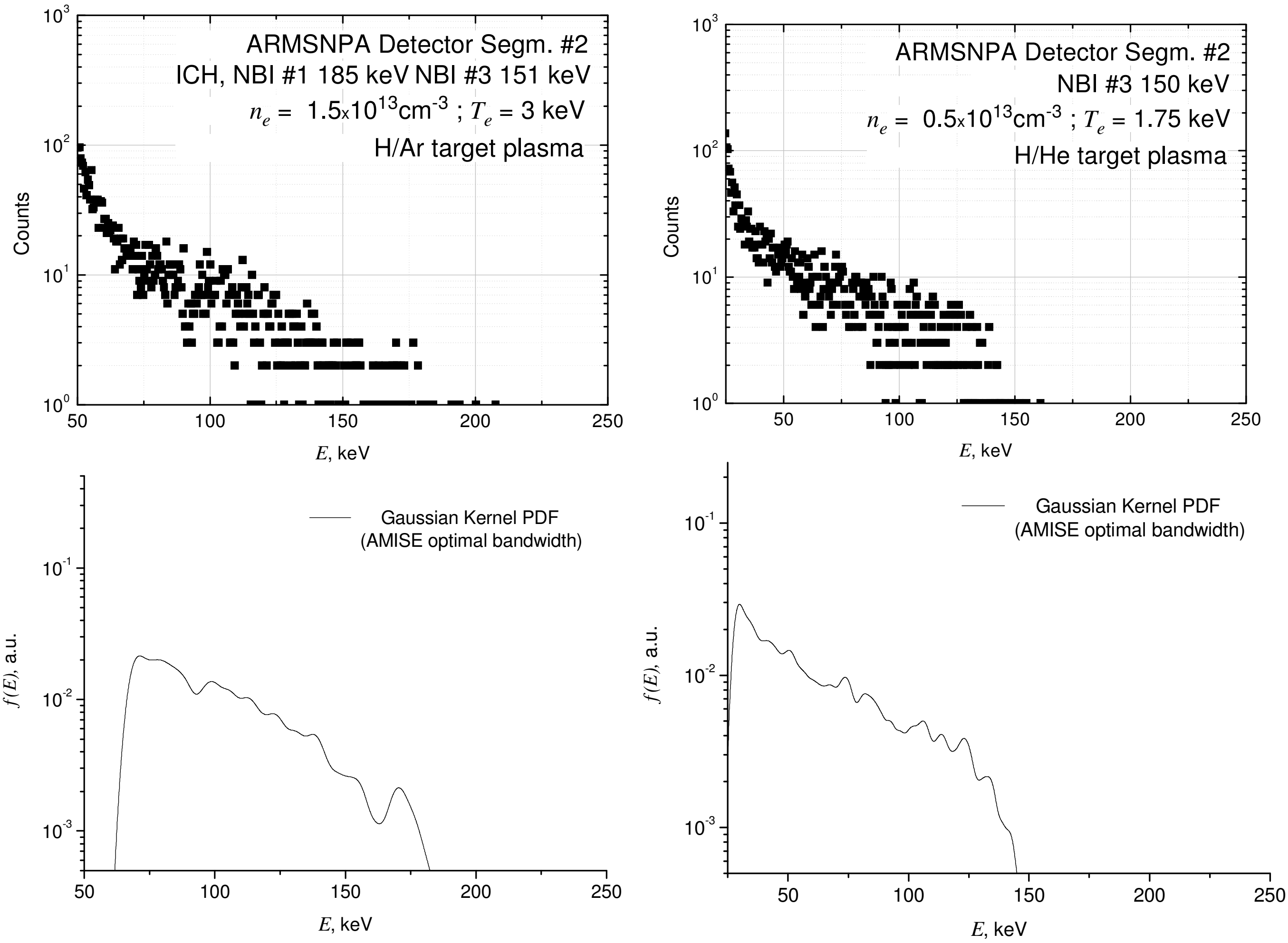

Fig. 2. Experimental H^0 energy spectra (upper) and PDF estimates (lower) for two different ion heating schemes.

$$a = \left(\frac{16\sqrt{2}}{5N}\right)^{1/7} \hat{\sigma} \quad \text{and} \quad b = \left(\frac{480\sqrt{2}}{105N}\right)^{1/9} \hat{\sigma}, \quad (17)$$

where $\hat{\sigma} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}\left(E_i - \overline{E}\right)^2}$, $\overline{E} = \frac{1}{N}\sum_{i=1}^{N} E_i$. (18)

Direct implementation of formula (15) is slow. An approximate fast calculation technique is given in [9].

5. Application to Experimental Data

These methods have been tested by reconstructing the probability density function from the generated pseudorandom number samples assuming Maxwellian and classical slowing down plasma ion energy distribution shapes for different temperatures and different slowing down times. The test results are shown in Fig. 1 (e) and (f). The analysis of passive chord-integrated experimental data obtained with the Angular-Resolved Multi-Sightline Neutral Particle Analyzer [1] on Large Helical Device is illustrated in Fig. 2. Kernel smoothing methods require a certain choice of the bandwidth parameter. An automatic choice described in Section 4 is preferable for routine data processing.

References

[1] E.A. Veshchev, T. Ozaki, et al., Rev. Sci. Instrum., **77**, 10F129 (2006).

[2] P.R. Goncharov, T. Ozaki, et al., Proc. 34th EPS Conf. Plasma Phys., P5.081 (Warsaw, 2007).

[3] S.K. Park, K.W. Miller, Comm. ACM, **31**, 1192 (1988).

[4] J.G. Cordey, M.J. Houghton, Nucl. Fusion, **13**, 215 (1973).

[5] A.W. Bowman, A. Azzalini, *Applied smoothing techniques for data analysis*, Clarendon (1997).

[6] M.P. Wand, M.C. Jones, *Kernel Smoothing*, Chapman and Hall, London (1995).

[7] V.A. Epanechnikov, Theory Probab. Appl., **14**, 153 (1969).

[8] S.J. Sheather, M.C. Jones, J. R. Statist. Soc. B, **53**, 683 (1991).

[9] V.C. Raykar, R. Duraiswami, *Very fast optimal bandwidth selection for univariate kernel density estimation*, University of Maryland, CS-TR-4774/UMIACS-TR-2005-73 (2006).