Pan-Spectrum Fitting Formula for Suprathermal Particles

Zixuan Liu1, Linghua Wang1, Robert F. Wimmer-Schweingruber2, Säm Krucker3,4, and Glenn M. Mason5

1School of Earth and Space Science, Peking University, Beijing, China, 2Institute of Experimental and Applied Physics, University of Kiel, Kiel, Germany, 3Space Sciences Laboratory, University of California, Berkeley, CA, USA, 4Institute of 4D Technologies, University of Applied Sciences Northwestern Switzerland, Windisch, Switzerland, 5Applied Physics Laboratory, Johns Hopkins University, Laurel, MD, USA

Abstract We propose a pan-spectrum fitting formula of suprathermal particles,

\[ J = A \times E^{-\beta_1} \left[ 1 + \left( \frac{E}{E_0} \right)^{\beta_1 - \beta_2} \right]^{\alpha-1}, \]

where \( J \) is the particle flux (or intensity), \( E \) is the particle energy, \( A \) is the amplitude coefficient, \( E_0 \) represents the spectral transition energy, \( \alpha (\geq 0) \) describes the sharpness and width of spectral transition around \( E_0 \), and the power-law index \( \beta_1 (\beta_2) \) gives the spectral shape before (after) the transition. This formula incorporates many commonly used spectrum functions as special cases. When \( \alpha \) goes to infinity (zero), this spectral formulabecomes the classical double-power-law (logarithmic-parabola) function. When both \( \beta_2 \) and \( E_0 \) approach infinity and \( \alpha \) is equal to 1, this formula can be simplified to the Ellison-Ramaty function. Under some other specific parameter conditions, this formula can be transformed to the Kappa or Maxwellian distribution. Considering the uncertainties in both particle intensity and energy, we improve the fitting method and fit this pan-spectrum formula well to the representative energy spectra of various suprathermal particle phenomena including SEPs (electrons, protons, 3He, and heavier ions), ESPs, bow-shocked electrons, solar wind suprathermal electrons, anomalous cosmic rays, and hard X-rays. Therefore, this pan-spectrum fitting formula would help us comparatively examine the properties of energy spectrum of different suprathermal particle phenomena typically with a single energy break.

1. Introduction

Suprathermal particles observed in space generally show a non-thermal energy spectrum that carries the crucial information on the origin, acceleration, and transportation of these particles. It is customary to characterize the spectral features by fitting the observed energy spectrum to a functional, parameterized formula. Previous studies suggested several spectrum formulae (e.g., Band et al., 2008; Ellison & Ramaty, 1985; Krucker et al., 2009; Lin & Schwartz, 1987) that, however, appear only suitable for fitting particular phenomenon/phenomena, respectively. For solar energetic electrons, hard X-rays (HXRs), and solar wind suprathermal particles (e.g., Dayeh et al., 2017; Krucker et al., 2009; Lin & Schwartz, 1987; Wang et al., 2006, 2015), their energy spectra are widely fitted to a single-power-law function, \( J(E) = A \times E^{-\beta} \), with a power-law index of \( \beta \), or a classic double-power-law (CDPL) function:

\[ J(E) = \begin{cases} A \times \left( \frac{E}{E_0} \right)^{-\beta_1}, & E < E_0 \\ A \times \left( \frac{E}{E_0} \right)^{-\beta_2}, & E > E_0, \end{cases} \]

where \( J \) is the particle flux (or intensity), \( A \) is the amplitude coefficient, \( E \) is the particle energy, \( E_0 \) is the break energy, and \( \beta_1 (\beta_2) \) is the power-law index before (after) the break. However, the CDPL function cannot characterize a smooth (not sharp) spectral transition.

For large solar energetic particle (SEP) events and energetic storm particle (ESP) events (e.g., Desai et al., 2004; Mewaldt et al., 2005), their particle spectra are often fitted to an Ellison-Ramaty (ER) function (Ellison & Ramaty, 1985), presumably expected from diffusive shock acceleration with finite shock size or lifetime. The ER function has a power-law form with an exponential cut-off at high energies:

\[ J(E) = A \times E^{-\beta} e^{-E/E_c}, \]

where \( E_c \) is the lifetime. The ER function has a power-law form with an exponential cut-off at high energies:
where \( E_c \) represents the cut-off energy. For large SEPs and Gamma-ray bursts (e.g., Band et al., 2008; Desai et al., 2016; Mewaldt et al., 2012), their particle spectra are sometimes fit well to a double-power-law band (BD) function defined as

\[
J(E) = \begin{cases} 
A \times E^{-\beta_1} e^{-E/E_B}, & E < (\beta_2 - \beta_1)E_B \\
A \times [(\beta_2 - \beta_1)E_B]^{2-\beta_2} E^{-\beta_2}, & E > (\beta_2 - \beta_1)E_B,
\end{cases}
\]  

where \( E_B \) is equivalent to \( E_c \) in the ER spectrum and \( \beta_1 (\beta_2) \) is the power-law index at very low energies (very high energies). Equation 3 shows that the BD formula is actually formed by an ER function at energies below a transition energy \( E_{tr} = (\beta_2 - \beta_1)E_B \) and a power-law function at energies above, with their first derivatives continuous at \( E_{tr} \). However, both the ER and BD functions cannot describe either a sharp spectral break or a spectral shape bending up at high energies.

For some suprathermal particles in space such as solar wind strahl/halo electrons (e.g., Livadiotis & McComas, 2010; Maksimovic et al., 2005; Tao et al., 2016), their spectral features could be described by the Kappa distribution (Vasyliunas, 1968):

\[
J(E) = \frac{n_0}{\pi m^2 c^3 (2kW_0)^{3/2}} \frac{\Gamma(\kappa + 1)}{\Gamma \left( \kappa - \frac{1}{2} \right) \Gamma \left( \frac{1}{2} \right)} \left( 1 + \frac{E}{kW_0} \right)^{-(\kappa+1)},
\]

where \( n_0 \) is the number density, \( W_0 \) is the effective thermal energy, \( \kappa > 3/2 \) is the Kappa index, and \( \Gamma(x) \) is the Gamma function. \( \kappa \) determines the power-law index of high-energy tail of Kappa distribution. When \( \kappa \) tends to infinity, the Kappa distribution becomes a thermal Maxwellian distribution.

In this paper, we propose a pan-spectrum formula with five parameters (section 2), in order to universally and objectively fit the energy spectrum of different suprathermal particle phenomena. Second, we improve the fitting method by considering the uncertainties in both particle intensity and energy (section 3). Finally, we utilize such a pan-spectrum fitting to well characterize the features of the representative energy spectra of various suprathermal particle phenomena including SEPs (electrons, protons, \(^3\)He, and heavier ions), ESPs, bow-shocked electrons, solar wind suprathermal electrons, anomalous cosmic rays (ACRs), and HXRs (Section 4).

### 2. Pan-Spectrum Formula

To construct a spectrum formula \( J(E) \) that can become a power-law function with a power-law index \( \beta_1 (\beta_2) \) at energies well below (above) a transition energy \( E_{tr} \), we would require its first derivative to satisfy

\[
\frac{d(\ln J)}{d(\ln E)} = \begin{cases} 
-\beta_1, & E \ll E_{tr} \\
-\beta_2, & E \gg E_{tr}.
\end{cases}
\]  

Arbitrarily, we come up with the following smooth tanh function (with continuous derivatives of any orders):

\[
\frac{d(\ln J)}{d(\ln E)} = -\frac{\beta_1 + \beta_2}{2} + \frac{\beta_1 - \beta_2}{2} \tanh \left[ \frac{\alpha(\ln E - \ln E_{tr})}{2} \right].
\]

After integrating Equation 6 over the energy \( E \), we obtain the formula of \( J(E) \) as

\[
J(E) = A \times E^{-\beta_1} \left[ 1 + \left( \frac{E}{E_{tr}} \right)^{\alpha} \right]^{\frac{\beta_1 - \beta_2}{2}},
\]  

where \( A \) is the amplitude coefficient and \( \alpha (>0) \) determines the sharpness and width of energy transition with a center at \( E_{tr} \). This proposed formula has five parameters: \( A, \beta_1, \beta_2, E_{tr}, \) and \( \alpha (>0) \). It accidentally appears to have a form close to the empirical “Nuker” law (Lauer et al., 1995) for fitting the brightness of galaxies as a function of their radius.

As shown in Figure 1a, the proposed formula (Equation 7) is a power-law of \( E^{-\beta_1} \) at very low energies and a power-law of \( E^{-\beta_2} \) at very high energies:

\[
J(E) = \begin{cases} 
A \times \left( \frac{E}{E_{tr}} \right)^{-\beta_1}, & \left( \frac{E}{E_{tr}} \right) \ll 1 \\
A \times \left( \frac{E}{E_{tr}} \right)^{-\beta_2}, & \left( \frac{E}{E_{tr}} \right) \gg 1.
\end{cases}
\]
connected by a smooth (for a finite $\alpha$) transition function at energies between. Such a smooth transition has a center at $E_0$, with a representative energy interval defined here as $[E_0 e^{-2/\alpha}, E_0 e^{2/\alpha}]$. When $\alpha$ increases towards infinity, the proposed formula becomes equivalent to the CDBL function (Equation 1) that has a sharp spectral break at $E_0$. On the other hand, when the power-law spectral index $\beta_1$ is less than (larger than) $\beta_2$, this formula describes a spectrum bending downwards (upwards) around $E_0$ (Figure 1c). When $\beta_1$ is equal to $\beta_2$, it becomes a single-power-law function.

Besides the single-power-law and CDPL functions, the proposed formula incorporates many spectrum formulae such as the ER function, Kappa distribution, and Maxwellian distribution as special cases. Therefore, it is hereinafter referred to as the “pan-spectrum” (PS) formula. For example, when both $\beta_2$ and $E_0$ approach...
infinity but their combination in the form of \( E_0 \left( \frac{\alpha}{\beta_0} \right)^2 \) remains finite, the PS formula becomes a ER-like function:

\[
\lim_{\beta_0 \to \infty} J(E) \propto E^{-\beta_0} e^{-(E/E_0)^2},
\]

where \( E_c = E_0 \left( \frac{\alpha}{\beta_0} \right)^2 \) represents the cutoff energy and \( \alpha \) determines the shape of exponential cutoff. When \( \alpha = 1 \), Equation 9 has the same form as the ER function (Figure 1d).

When \( \alpha \) approaches 0, the PS formula can be simplified to a logarithmic parabola (Figure 1e):

\[
\lim_{\alpha \to 0} J(E) \propto E^{-1} e^{-(E/E_0)^2},
\]

with an infinite transition energy interval of \([0, + \infty)\). This logarithmic parabola function cannot be simply characterized by the parameters themselves.

When \( \beta_1 = -1 \), the PS formula can be transformed to the isotropic form of generalized Lorentzian function (e.g., Hu et al., 2017; Quershi et al., 2003; Randol & Christian, 2014):

\[
J(E)\bigg|_{\beta_1 = -1} \propto E \left( 1 + \left( \frac{E}{\beta_2 W_0} \right)^2 \right)^{-\frac{\beta_1 + 1}{2}},
\]

where \( W_0 = \frac{E_0}{\beta_1} \) is equivalent to effective thermal energy. When \( \alpha = 1 \), Equation 11 can be further converted to the Kappa distribution (Figure 1f):

\[
J(E)\bigg|_{\beta_1 = -1} \propto E \left( 1 + \frac{E}{\beta_2 W_0} \right)^{-\frac{(\beta_1 + 1)}{2}},
\]

where \( \beta_1 \) is equivalent to the Kappa index. Moreover, when both \( \beta_1 \) and \( E_0 \) also go to infinity, Equation 12 can be transformed to the Maxwellian distribution (Figure 1g):

\[
J(E)\bigg|_{\beta_1 = -1} \propto E e^{-\frac{E}{T_m}},
\]

where \( E_{th} = \lim_{\beta_1 \to \infty, \beta_2 \to \infty} \frac{E_0}{\beta_1} \) is the thermal energy.

3. Fitting Method

We utilize the nonlinear least-square algorithms to fit a series of \( n \) data points \((x_i, y_i)\) to a parameterized function, \( y = f(x, \mathbf{a}) \), where \( \mathbf{a} = (a_1, a_2, \ldots, a_m) \) is a vector (or a set) of \( m \) unknown parameters. In this method, the best fit is determined by minimizing the reduced chi-square statistic (e.g., Bevington & Robinson, 2003). Given a fixed \( n \), the smaller the value of reduced chi-square, the better the fit (West et al., 2012).

If the \( x_i \) are precise and the \( y_i \) are not exact, the reduced chi-square statistic is the sum of normalized residuals defined as

\[
\chi^2_n(a) = \frac{1}{n-m} \sum_{i=1}^{n} \left( \frac{y_i - f(x_i, \mathbf{a})}{\sigma_{y_i}} \right)^2,
\]

where \( n \) and \( m \) are, respectively, the number of data points and the number of parameter, the denominator of \( n - m \) is the statistical degrees of freedom, and \( \sigma_{y_i} \) is the standard deviation of \( y_i \). In practice, the \( \sigma_{y_i} \) are generally assigned the value of the measurement uncertainties of \( y_i \), that is, \( \sigma_{y_i} = \Delta y_i \). If the \( y_i \) obey a normal or Gaussian distribution and the \( \sigma_{y_i} \) are reasonably estimated, \( \chi^2_n \) would be close to 1. If the \( \sigma_{y_i} \) are significantly overestimated, \( \chi^2_n \) would be much less than 1 (Bevington & Robinson, 2003).

If both \( x_i \) and \( y_i \) are not precise, the reduced chi-square statistic can have the form defined as

\[
\chi^2_n(a) = \frac{1}{n-m} \sum_{i=1}^{n} \left( \frac{y_i - f(x_i, \mathbf{a})}{\sigma_{y_i}^2 + \sigma_{x_i}^2 + \sigma_{y_i}^2} \right)^2,
\]
where $\sigma_i$ is the standard deviation of $x_i$, and $f'_i = \frac{\partial f}{\partial x_i}$. If $\sigma_i$ and/or $\sigma_x$ are significantly overestimated, $\chi^2(a)$ would be much less than 1.

When fitting to the measured particle energy spectrum, we generally assign the channel center energy to $x_i$ and the average flux (or intensity) to $y_i$, for a given energy channel $i$. Since the channel-average flux usually does not correspond exactly to the channel center energy (i.e., $x_i$ is not precisely known as well), we utilize this improved $\chi^2$ as a goodness-of-fit index in this paper. Note, however, that the $\chi^2$ is usually not an index for model comparison or selection (e.g., West et al., 2012).

We apply the quasi-Newton method (e.g., Broyden, 1970) to find the minimum of $\chi^2(a)$ in the parameter space and obtain the corresponding best fit with a fitted parameter vector $a^f$ (see Figure 2). If the $x_i$ and $y_i$ obey a normal distribution, then $\chi^2 = (n - m) \times \chi^2$ would satisfy the chi-square probability distribution with the $n - m$ degrees of freedom and the parameter vector $a$ is subjected to a multivariate normal distribution. Thus, the covariance matrix $C$ of $a$ can be calculated as follows (Press et al., 1992):

$$C = \left( \frac{H}{2} \right)^{-1},$$

where $H$ is the Hessian matrix of $\chi^2$, that is, $H_{ij} = (n - m) \frac{\partial^2 f}{\partial a_i \partial a_j}$. For the fitted parameters $a^f$, we use their standard deviation, defined as $\delta a_i^{fit} = \sqrt{C_{ii}}$ (Press et al., 1992), to estimate their uncertainties.

For the PS formula with five parameters (Equation 7), $y = J(E)$, and $a = (A, \beta_1, \beta_2, E_0, \alpha)$. Given a parameter vector $a = (a^1, a^2, a^3, 3\text{ keV}, 2)$, we construct a test set of 33 sample points $(E_i, J_i)$, where $E_i = E_0 + \bar{E}i, J_i = J_0 + J_i$, $E_0$ and $J_0$ are equally spaced on a logarithmic scale in energies from 0.1 to 100 keV, $J_i = J(E_0, a)$, and $\bar{E}$ and $J_i$ are randomly selected, respectively, according to a standard deviation of $\sigma_{E_0} = 0.1E_0$ and $\sigma_J = 0.1J_0$. Figure 2 shows the best fit to these sample points with a fitted parameter vector $a^f = (a^{1\times 2}, 2.01.5, 91, 3.1 \text{keV}, 2, 23)$, consistent with $a$ (indicated by asterisks in Figures 2b–2e) within the estimated uncertainties. The $a^f$ with the estimated uncertainties is also consistent with the confidence regions indicated by the contours of $\chi^2$ for 28 degrees of freedom.

In statistical practice (e.g., Hamby, 1994; Press et al., 1992), Monte Carlo simulation can be used to characterize the uncertainties of parameter estimation in a very precise way, by obtaining the probability distribution of output parameters from fitting to random sampling input data sets. Given the same parameter vector $a = (a^1, a^2, a^3, 3\text{ keV}, 2)$, here, we randomly generate 1,000 test sets of 33 sample points $(E_i, J_i)$ with a relative Gaussian noise of 0.1 in both energy and flux and obtain a distribution of minimal $\chi^2$ and fitted parameters from fitting to these 1,000 test sets. Figure 3a shows that the probability distribution function of simulated minimal $\chi^2$ (solid line) peaks at 1.0 and agrees with the ideal reduced chi-square distribution for

![Figure 2](image-url)
Figure 3. Fitting results of 1,000 test spectra that are randomly generated with relative errors of 0.1 in both energy and flux, for the same initial parameter vector \( \bar{a} \) in Figure 2. (a) The probability distribution function (PDF) of simulated minimal \( \chi^2 \) (solid line), compared with the ideal reduced chi-square distribution for 28 degrees of freedom (dashed line). (b–g) Scatter plots between four parameters from fitting to the 1,000 test spectra. The asterisks indicate the initial parameter vector, and the red bars denote the parameter uncertainties shown in Figure 2. The green horizontal and vertical solid lines denote the standard deviations of the simulated distribution of parameters.

Figure 4. Best fits to the representative SEP electron (top) and proton (bottom) spectra, using the PS (red), CDPL (purple), ER (blue) and BD fitting formulae. The black dots with error bars show the observations with uncertainties. For the proton data, we assume a relative uncertainty of 0.2 and 0.1, respectively, in flux and energy.
Figure 5. Best fits to the the representative energy spectra of SEP $^3$He (a), ACR He (b), ESP Fe (c), bow-shocked electrons (d), upstream electron event (e), HXR flare (f), solar wind suprathermal electrons (g), solar wind halo electrons (h) and simulated thermal electrons (i), using the PS (red), CDPL (purple), ER (blue) and BD fitting formulae. In panel (i), The test data points of thermal electrons are generated from a Maxwellian distribution with $E_{th} = 50$ eV.

28 degrees of freedom (dashed line). Figures 3b–3g plot the scatter diagrams between four fitted parameters ($\beta_1, \beta_2, E_0, \alpha$) in simulations, showing a positive (correlation coefficient $CC > 0.5$) correlation between $\beta_1$ and $\alpha$ and between $\beta_2$ and $E_0$ and a negative ($CC < -0.5$) correlation between $\beta_2$ and $\alpha$. Figures 3b–3g also show that the standard deviations of the simulated distribution of parameters (shown as green bars) are similar to the parameter uncertainties (defined as $\delta a_i^{(j)} = \sqrt{C_{ii}}$ in our fitting method) calculated from fitting to only one test set (red bars in Figures 2 and 3).

4. Fits to Suprathermal Particle Energy Spectra

We apply the fitting method described in section 3 to the representative particle energy spectra of various suprathermal particle phenomena measured in space, after considering the uncertainties in both particle intensity $J$ and energy $E$. There are two independent sources of uncertainties: the statistical uncertainties of $J$ (that can be approximately regarded as an normal distributed uncertainty) and the systematic uncertainties of $E$ (that should be affected by many factors including the instrumental resolution and response and the spectral shape within the energy channel). In a simple way, here we assign the energy width of channel to $\sigma_{E_i}$. Note that the energy channel width is usually much larger than the measurement uncertainty of $E_i$, and it can be regarded as the upper limit of $\sigma_{E_i}$.

For a quasi-quantitative comparison among different spectrum fitting models including PS, CDPL, ER, and BD, we use the expected cross-validation index (ECVI) as a model selection index (e.g., West et al., 2012):

$$\text{ECVI} = \frac{n - m}{n - 1} \min \left( \chi^2_i \right) + \frac{2m}{n}. \quad (17)$$
Table 1
Fitted spectral parameters of Figures 3 and 4

|       | PS            | CDPL           | ER     | BD         |
|-------|---------------|----------------|--------|-----------|
|       | $\beta_1$     | $\beta_2$      | $E_{\gamma}$ | $a$       | $E_1$     | $\beta_1$ | $\beta_2$ | $E_{\gamma}$ |
| Figure 4 |                |                |        |            |           |          |          |             |
| a     | $1.9 \pm 0.1$ | $3.8 \pm 0.9$  | $73 \pm 50$ keV | $6 \pm 21$ | $1.9 \pm 0.1$ | $37 \pm 0.5$ | $66 \pm 27$ keV | $1.9 \pm 0.1$ | $111 \pm 35$ keV | $1.8 \pm 0.1$ | $41 \pm 1.4$ | $96 \pm 45$ keV |
| b     | $192 \pm 0.05$| $3.8 \pm 0.2$  | $71 \pm 11$ keV | $>10$      | $1.93 \pm 0.04$| $38 \pm 0.2$  | $74 \pm 10$ keV | $1.90 \pm 0.04$| $125 \pm 9$ keV | $1.79 \pm 0.06$| $4.0 \pm 2.2$ | $84 \pm 12$ keV |
| Figure 5 |                |                |        |            |           |          |          |             |
| a     | $1.1 \pm 0.1$ | $4.5 \pm 0.4$  | $41 \pm 10$ MeV/n | $1.9 \pm 0.8$ | $1.19 \pm 0.03$| $41 \pm 0.2$  | $36 \pm 3$ MeV/n | $1.14 \pm 0.04$| $39 \pm 4$ MeV/n | $0.98 \pm 0.04$| $4.3 \pm 0.2$ | $25 \pm 3$ MeV/n |
| b     | $108 \pm 0.05$| $4.5 \pm 0.2$  | $40 \pm 5$ MeV/n | $2.1 \pm 0.5$ | $1.19 \pm 0.02$| $40.8 \pm 0.06$| $35 \pm 1$ MeV/n | $1.29 \pm 0.02$| $69 \pm 2$ MeV/n | $0.97 \pm 0.03$| $4.3 \pm 0.1$ | $25 \pm 2$ MeV/n |

*The parameters listed in the row are estimated by neglecting the energy uncertainties. *Only the lower limit of $\beta_1$ is available, since $E_{\gamma} = 0.5 \times \beta_2$ is larger than the data energy range. *These parameters are not applicable, since the data are best fitted to a single-power-law. *Failed fitting.
Smaller ECVI values could indicate better model fit. In addition, the spectral transition energy $E_t$ is defined as $E_{0_t}$, $E_{01}$, $E_{02}$, $(\beta_1 - \beta_2)E_{0p}$, respectively, for the PS, CDPL, ER, and BD fitting.

In Figure 4, the top (bottom) panels compare the best fits to the SEP electron (proton) spectrum reported by Krucker et al. (2009) (by Mewaldt et al., 2012), using the PS, CDPL, ER, and BD fitting formulae. For the Krucker et al. (2009) electron spectrum, all four fittings provide good fits, indicated by a small ECVI value (0.5–0.7), and they have the fitted power-law indexes (when applicable) consistent with each other. The fitted $E_{0_t}$ is consistently reasonable from the PS, CDPL and ER fittings, but it appears to be significantly overestimated from the BD fitting. For the Mewaldt et al. (2012) proton spectrum, the PS, CDPL, and BD fittings tend to give good fits with a small ECVI value (∼0.7–1.0), while the ER fitting provides bad fits with a large ECVI value (∼1.9). The PS and CDPL fittings give consistent $E_{0_t}$ and power-law indexes below/above $E_{tr}$, while the BD fitting exhibits similar power-law indexes but a likely overestimated $E_{0_t}$. In addition, the PS fitting provides a totally new parameter $a$ to characterize the shape and energy width of spectral transition. The fitted $a$ is around 6 and 2, respectively, for the representative SEP electron and proton spectra shown in Figure 4.

Figures 5a–5g show the fitting results to the representative spectra of ESP Fe ions (Desai et al., 2004), ACR He ions (Cummings et al., 2002), SEP 3He ions (Mason et al., 2002), bow-shocked electrons (Liu et al., 2000), an “upstream electron event” near the bow shock (Liu et al., 2000), HXRs (Krucker et al., 2007), and solar wind suprathermal electrons at ~0.4–200 keV (Yang et al., 2019), using the PS (red), CDPL (purple), ER (blue), and BD (green) formulae. Table 1 lists the fitted parameters of these spectra. Among the four fittings, only the PS provides good fits (indicated by a small ECVI value), as well as good estimates of $E_{0_t}$, to all these suprathermal particle spectra. Figures 5h–5i also indicate that the PS fitting can give good fits to the particle energy spectrum in the Kappa distribution (such as solar wind halo/strahl electrons; Tao et al., 2016) and a thermal Maxwellian distribution.

In most cases shown in Figures 4 and 5, the fitted parameters sometimes have large uncertainties and the values of $\chi^2$ are much less than 1, likely due to the overestimate of energy uncertainty as the energy channel width and/or the limited number of data points. If the energy uncertainties are set to 0, the uncertainties of fitted parameters can decrease significantly (see Table 1).

5. Summary and Discussion

We propose a PS fitting formula for suprathermal particles measured in space, $J = A \times E^{-\beta} \left[1 + \left(\frac{E}{E_{0}}\right)^{\alpha}\right]^{\frac{\beta_1 - \beta_2}{2}}$ (Equation 7), with five parameters: the amplitude coefficient $A$, spectral transition energy $E_{0_t}$, power-law index $\beta_1$ ($\beta_2$) before (after) the transition, and transition shape parameter $a$ (>0). This PS formula incorporates the single-power-law, CDPL and ER functions, as well as the Kappa and Maxwellian distributions, as special cases. Considering the uncertainties both in $J$ and $E$, we improve the fitting method and fit the PS formula well to the representative energy spectra of various suprathermal particle phenomena including SEPs (electrons, protons, 3He, and heavier ions), ESPs, bow-shocked electrons, solar wind suprathermal electrons, ACRs, and HXRs. Thus, the PS fitting would help us comparatively examine and compare the properties of energy spectrum of different suprathermal particle phenomena and understand the nature of their origin, acceleration, and transportation.

The spectral transition carries important information on the particle acceleration and/or transportation, but its shape and energy width are poorly studied. In the PS fitting formula, $E_{0_t}$ and $a$ together can well describe the features of spectral transition. In particular, $a$ is a new parameter to qualitatively determine the shape and width of spectral transition. A larger $a$ indicates a narrower and sharper transition in the particle spectrum. The energy interval of spectral transition is defined here as $[E_{0_t}e^{-2/\alpha}, E_{0_t}e^{2/\alpha}]$, with a center at $E_{0_t}$ in logarithmic scale. During this interval (Figure 1a), the spectral slope in the log-log scale ranges from $-(0.88\beta_1 + 0.12\beta_2)$ to $-(0.12\beta_1 + 0.88\beta_2)$, with a center value of $-(\beta_1 + \beta_2)/2$ occurring at $E_{0_t}$. Thus, the PS fitting can help us comprehensively study the features of spectral transition.

The PS formula incorporates many commonly used spectral functions as special cases (Figure 1). For example, when $a$ tends to infinity (zero), the PS formula becomes the CDPL (logarithmic-parabola) function. When both $\beta_2$ and $E_{0_t}$ tend to infinity and $a$ is equal to 1, this formula can be simplified to the ER function. Under other specific parameter conditions, this formula can be transformed to the isotropic form of generalized Lorentzian distribution, Kappa distribution, or Maxwellian distribution. The fitting results show
that among the PS, CDPL, ER, and BD fittings (Figures 4 and 5), only the PS fitting provide good fits to all the shown energy spectra of suprathermal particles including SEPs, ESPs, bow-shocked electrons, solar wind suprathermal electrons, ACRs, and HXRs. Therefore, the PS fitting formula would help us quantitatively compare the spectral features of different suprathermal particle phenomena. Note that the minimum number of data points would be around 10 to avoid over-fitting and enable a reasonable estimate of parameter uncertainties, since there are five parameters in this fitting model.

In fitting practice, people assign the average flux (or intensity) measured in an energy channel to \( J \) and its uncertainties to \( \sigma_J \), while they assign the channel center energy to \( E \) but generally ignore \( \sigma_E \). However, the uncertainties of \( E \) are not negligible, since the channel-average flux usually does not correspond exactly to the channel center energy. In this paper, we improve the form of \( \chi^2 \) by including both uncertainties in \( J \) and \( E \) (Equation 14) and utilize the quasi-Newton method (e.g., Broyden, 1970) to find the minimum of \( \chi^2 \) in the parameter space. We also use the covariance matrix of parameter vector (Equation 15) to estimate the uncertainties of fitted parameters.

In spectrum fitting, we assign the energy width of channel to \( \sigma_E \) and treat the energy uncertainties as random errors in a simply way. Note that the uncertainties of \( E \) may be highly correlated and should be affected by many factors including the instrumental resolution and response, the spectral shape within the energy channel, and so forth. We will improve the estimate of \( \sigma_E \) in future. Also note that the PS fitting model is applicable for studying the particle spectra with no more than one energy break/transition.

We independently derive the PS formula of suprathermal particles in a mathematical way, although it accidentally appears to have a form close to the empirical “Nuker” law (Lauer et al., 1995) that fits to the brightness of galaxies as a function of their radius. Then we are able to quantitatively define an energy transition range of particle spectrum. In addition, we show mathematically that the PS formula incorporates many commonly used spectral functions. Using this PS fitting, therefore, we are able to consistently compare the spectral features (e.g., spectral transition and spectral indexes) of different suprathermal particle phenomena, in order to investigate the relationship between the origin/acceleration of these phenomena (e.g., solar energetic electrons and \(^3\)He-rich ions). Moreover, we can quantitatively examine the interplanetary evolution of the spectral shape of solar suprathermal particles in future, combining the in situ measurements from Solar Orbiter (Müller et al., 2013), Parker Solar Probe (Fox et al., 2016), Wind, and ACE.

Data Availability Statement

All the spacecraft data used in this manuscript are available through Krucker et al. (2009), Mewaldt et al. (2012), Desai et al. (2004), Cummings et al. (2002), Mason et al. (2002), Liu et al. (2000), Krucker et al. (2007), Yang et al. (2019), and Tao et al. (2016).

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