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Physical interpretation of the Padé approximation of the plasma dispersion function

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Abstract. It is shown that using Padé approximants in the evaluation of the plasma dispersion function Z for a Maxwellian plasma is equivalent to the exact treatment for a plasma described by a 'simple-pole distribution', i.e. a distribution function that is a sum of simple poles in the complex velocity plane (v plane). In general, such a distribution function will have several zeros on the real v axis, and negative values in some ranges of v. This is shown to be true for the Padé approximant of Z commonly used in numerical packages such as WHAMP. The realization that an approximation of Z is equivalent to an approximation of $f(v)$ leads the way to the study of more general distribution functions, and we compare the distribution corresponding to the Padé approximant used in WHAMP with a strictly positive and monotonically decreasing approximation of a Maxwellian.

1. Introduction

Dispersion relations are fundamental for understanding the linear properties of homogeneous plasmas. To derive a dispersion relation in kinetic plasma theory, a distribution function for each particle species is introduced to describe the unperturbed plasma. As an equilibrium plasma is described by a Maxwellian velocity distribution, this distribution is widely used in textbooks as well as in research papers. Even in cases where the plasma is clearly non-Maxwellian, sums and products of Maxwellians are often used (see e.g. Maggs 1976; Gustafsson et al. 1990). The reason for this seems to be more that already-established and well-known results for the Maxwellian distribution can be used, rather than a belief that a combination of Maxwellians actually gives an optimal description of the situation. However, it is also possible to model the plasma without reference to the Maxwellian, and the best known way is probably to use the Lorentzian or kappa distribution (Summers and Thorne 1991). In this paper, we want to shed light on an approximation frequently used in the wave theory of Maxwellian plasmas by comparison with results obtained by using another class of distribution functions, the simple-pole distributions introduced by Löfgren and Gunell (1997).

The Maxwellian distribution can be written

$$f_{\mathrm{M}}(v) = \frac{1}{\sqrt{\pi}} e^{-v^2}, \tag{1.1}$$

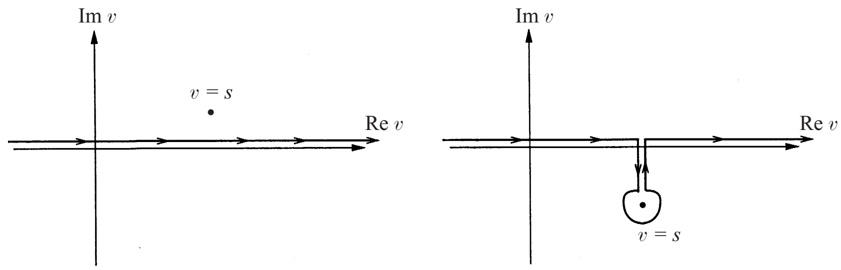

Figure 1. The 'Nautilus convention'. The integration path must always go below the pole at $v = s$.

where the normalized velocity v is related to the particle velocity u by $u = vv_t$, $v_t = (2K_B T/m)^{1/2}$ is the thermal velocity, K_B is Boltzmann's constant and T is the temperature. The derivation of a dispersion relation for waves in a plasma with Maxwellian particle distribution leads to the plasma dispersion function (Fried and Conte 1961)

$$Z(s) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-v^2}}{v-s} dv, \quad (\mathrm{Im}\, s > 0), \tag{1.2}$$

or some equivalent integral. For instance, the dispersion relation for an unmagnetized plasma with M particle species is

$$k^2 = \sum_{\alpha=1}^{M} \frac{\omega_{p\alpha}^2}{v_{t\alpha}^2} Z'_\alpha(\omega/k). \tag{1.3}$$

Corresponding expressions for magnetized plasmas can readily be found in standard textbooks (e.g. Brambilla 1998). Care must be taken to treat the pole at $v = s$ correctly when analytically continuing the definition (1.2) into the lower complex v plane, leading to the 'Nautilus convention' shown in Fig. 1 (cf. Swanson 1989) and the extended definition (cf. Brambilla 1998, p. 107)

$$Z(s) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-v^2}}{v-s} dv + \begin{cases} 0 & (\mathrm{Im}\, s > 0), \\ i\sqrt{\pi} e^{-s^2} & (\mathrm{Im}\, s = 0), \\ 2i\sqrt{\pi} e^{-s^2} & (\mathrm{Im}\, s < 0), \end{cases} \tag{1.4}$$

valid for all complex s.

The integrand in (1.4) does not have any poles except $v = s$, and goes to infinity as $v \to \pm i\infty$. In contrast to the class of distribution functions to be considered in Sec. 2, the integral cannot be calculated using the residue theorem, and $Z(s)$ must in general be found by approximate or numerical methods.

In addition to the obvious interest in studies of non-equilibrium plasmas, there may thus be another reason to consider non-Maxwellian distributions: the desire to simplify computations. Other distributions may allow analytical calculation of the integral corresponding to (1.4), which we define as the generalized plasma dispersion function

$$Z_G(s) = \int_{-\infty}^{\infty} \frac{f(v)}{v-s} dv \quad (\mathrm{Im}\, s > 0) \tag{1.5}$$

In Sec. 2, we discuss the 'simple-pole distribution', for which we derive an analytical expression for $Z_G(s)$. In Sec. 3, we compare this function with the Padé approximation used to calculate $Z(s)$, for example by Rönnmark (1982). It is found that the Padé approximation of $Z(s)$ is identical to an exact expression for $Z_G(s)$ for a unique simple-pole distribution, which turns out to be piecewise-negative. Some other possible approximations of the Maxwellian distribution are discussed and compared with the Padé approximation in Sec. 4. Finally, we discuss the results in Sec. 5.

2. The simple-pole distribution

We model the distribution function of a plasma particle species as a sum of simple poles in the complex velocity plane,

$$f(v) = \sum_j \frac{a_j}{v-b_j}, \tag{2.1}$$

which we call the 'simple-pole distribution'. This was introduced by Löfgren and Gunell (1997), who also derived the corresponding dispersion relation in an unmagnetized plasma. Nakamura and Hoshino (1998) have used a related approach for studying weakly relativistic effects on waves in a magnetized plasma.

In general, the distribution function (2.1) will be complex-valued for real v. To restrict to real values, we shall always assume that each pole $v = b$ with residue a has a counterpart $v = b^*$ with residue a^*, where * denotes complex conjugation, so that

$$f(v) = \sum_j \left(\frac{a_j}{v-b_j} + \frac{a_j^*}{v-b_j^*}\right). \tag{2.2}$$

To further ensure that $f(v) \geqslant 0$, it is for example possible to square the term in parentheses. Some other possibilities for writing distribution functions in terms of simple poles have been considered by Tjulin (1999). We shall not consider this issue here.

We may note that if the condition

$$\mathrm{Re}\left(\sum_j a_j\right) = 0 \tag{2.3}$$

is fulfilled, we can see that for $|v| \to \infty, f(v)$ goes to zero at least as fast as $1/|v|^2$ in all directions in the complex v plane. The condition (2.3) is satisfied for all functions $f(v)$ of the type (2.1) that are even ($f(v) = f(-v)$). These are the only functions that we shall consider from here on.

It has now been shown that it is possible to close the integration contour in (1.5) by a semicircle to infinity in the lower (Fig. 2) or upper half-plane,

$$Z_G(s) = \int_{-\infty}^{\infty} \sum_j \frac{a_j}{v-b_j}\frac{1}{v-s}\,dv = \oint_C \sum_j \frac{a_j}{v-b_j}\frac{1}{v-s}\,dv. \tag{2.4}$$

The integral may now be calculated by the residue theorem, yielding

$$Z_G(s) = -2\pi i \sum_{b_j \in \mathbb{L}} \frac{a_j}{b_j - s}, \tag{2.5}$$

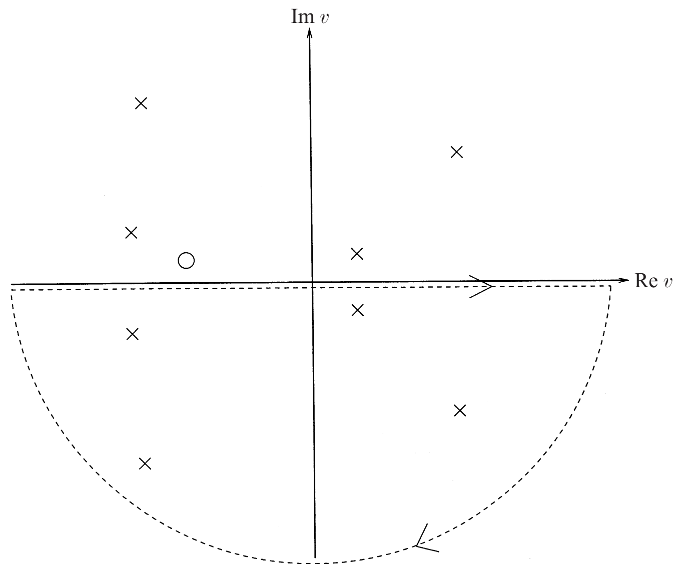

Figure 2. The integration contour in (2.5). The poles in the distribution function are denoted by crosses and the pole at $v = s$ by a circle.

where the summation is over all poles b_j of $f(v)$ that lie in the lower complex half-plane $\mathbb{L}$. Note that for an analytic continuation of $Z_G(s)$ to $\operatorname{Im} s < 0$, the pole at $v = s$ should not be included in the sum (Fig. 2). As the sum in (2.5) refers only to the poles of $f(v)$, it is clear that this requirement is satisfied. Thus (2.5) is a valid expression for $Z_G(s)$ for all s, and there is no need to treat special cases as in (1.4).

Instead of closing the contour C in the lower half-plane, we might just as well have closed it in the upper half-plane. In that case, the contribution from the pole at $v = s$ must be included in the sum. It is straightforward to show that the expression obtained in this way is equivalent to (2.5).

3. Padé approximation of $Z(s)$

As noted above, the integral in the definition (1.4) of $Z(s)$ for a Maxwellian distribution cannot be evaluated analytically. Some sort of approximation is therefore needed. Martín and Gonzáles (1979) introduced a Padé method, which was extended and used by Rönnmark (1982) in the widely used software package WHAMP. The Padé approximant used by Rönnmark can be written as

$$Z_P(s) = \sum_j \frac{A_j}{s - B_j}, \tag{3.1}$$

with coefficients A_j and B_j listed in Table 1 (Rönnmark 1982).

Comparing the expressions for $Z_G(s)$ and $Z_P(s)$ in (2.5) and (3.1), it is obvious that the Padé approximant of $Z(s)$ corresponds to an exact $Z_G(s)$ for a plasma described by a simple-pole distribution (2.1). We may call this particular simple-pole distribution function $f_P(v)$, and we shall now derive the poles b_j and residues a_j describing it.

Table 1. The coefficients A_j and B_j used by Rönnmark (1982).

j	A_j
1	$-0.01734012457471826-0.04630639291680322i$
2	$-0.01734012457471826+0.04630639291680322i$
3	$-0.7399169923225014+0.8395179978099844i$
4	$-0.7399169923225014-0.8395179978099844i$
5	$5.840628642184073+0.9536009057643667i$
6	$5.840628642184073-0.9536009057643667i$
7	$-5.583371525286853-11.20854319126599i$
8	$-5.583371525286853+11.20854319126599i$
j	B_j
1	$2.237687789201900-1.625940856173727i$
2	$-2.237687789201900-1.625940856173727i$
3	$1.465234126106004-1.789620129162444i$
4	$-1.465234126106004-1.789620129162444i$
5	$0.8392539817232638-1.891995045765206i$
6	$-0.8392539817232638-1.891995045765206i$
7	$0.2739362226285564-1.941786875844713i$
8	$-0.2739362226285564-1.941786875844713i$

As all poles in (3.1) are in the lower half of the complex plane (Table 1), it is possible to write

$$Z_{\mathrm{P}}(s)=\sum_j \frac{A_j}{s-B_j}=\sum_{B_j\in\mathbb{L}} \frac{A_j}{s-B_j}. \tag{3.2}$$

From comparison with (2.5), it is clear that this corresponds to an integral

$$\begin{aligned} Z_{\mathrm{P}}(s) &= \sum_{B_j\in\mathbb{L}} \frac{A_j}{s-B_j} = -2\pi i\left(\frac{1}{2\pi i}\sum_{B_j\in\mathbb{L}}\frac{A_j}{B_j-s}\right) \\ &= \int_{-\infty}^{\infty}\frac{1}{2\pi i}\left(\sum_j \frac{A_j}{v-B_j}+G(v)\right)\frac{1}{v-s}\,dv, \end{aligned} \tag{3.3}$$

where $G(v)$ is an unspecified function that (i) may only have poles in the upper complex half-plane and (ii) goes to zero when v goes to infinity for the integral to be finite. These requirements uniquely identify $G(v)$, and we get

$$f_{\mathrm{P}}(v)=\frac{1}{2\pi i}\sum_j\left(\frac{A_j}{v-B_j}-\frac{A_j^*}{v-B_j^*}\right). \tag{3.4}$$

This expression is unique in the sense that it is the only physically acceptable (in the sense of being real-valued for real v) simple-pole distribution function that has a plasma dispersion function exactly equal to (3.1). The use of the Padé approximant of $Z(s)$ is thus equivalent to an unique approximation of the Maxwellian by a simple-pole distribution. In other words, a simple-pole distribution is implicitly assumed when using the Padé approximant.

We may note that there is no guarantee that the corresponding simple-pole distribution $f_{\mathrm{P}}(v)$ is positive. Indeed, Fig. 3 shows that the function $f_{\mathrm{P}}(v)$, in this case, is piecewise-negative, and also has regions of $df_{\mathrm{P}}(v)/dv > 0$. The consequences of this will be discussed in the next section.

4. Comparison of distribution functions

We shall now compare the distribution function f_{P} with the Maxwellian, and with another simple-pole approximation of the Maxwellian introduced by Löfgren and Gunell (1997). They wrote the Maxwellian (1.1) as

$$f_{\mathrm{M}}(v) = \frac{1}{\sqrt{\pi}}\frac{1}{e^{v^2}} = \frac{1}{\sqrt{\pi}}\frac{1}{\sum_{j=0}^{\infty}\frac{v^{2j}}{j\,!}}, \tag{4.1}$$

using the common Taylor expansion of e^{v^2} and truncating at some arbitrary $j = N$. The resulting function obviously is positive on the real axis and monotonically decreasing, thus overcoming the principal difficulties with f_{P}. The denominator is a polynomial of v of degree $2N$ with equally many distinct roots, so $f_{\mathrm{M}}^{N}(v)$ has $2N$ simple poles $v = b_j$ in the complex v plane. By solving the polynomial equation obtained by putting the denominator equal to zero, it is straightforward to find the poles b_j and their corresponding residues a_j. We thus get a simple-pole distribution

$$f_{\mathrm{M}}^{(N)}(v) = \frac{1}{K}\sum_{j=1}^{N}\frac{a_j}{v-b_j}, \tag{4.2}$$

where

$$K = \int_{-\infty}^{\infty} f_{\mathrm{M}}^{(N)}(v)\,dv = -2\pi i \sum_{b_j\in\mathbb{L}} a_j \tag{4.3}$$

has been introduced in order to ensure unit value of the zeroth-order moment.

We shall also compare these distribution functions with the one-dimensional kappa distribution (or generalized Lorentzian) (Summers and Thorne 1991), which is of the form

$$f_{\kappa}(v) = K\left(1+\frac{v^2}{\kappa}\right)^{-\kappa}. \tag{4.4}$$

K is chosen so that the zeroth-order moment attains unit value. Clearly, $f_{\kappa}(v) \to f_{\mathrm{M}}(v)$ as $v \to \infty$.

Using the coefficients A_j and B_j used by Rönnmark (1982) in the WHAMP code (Table 1), we plot the distribution function $f_{\mathrm{P}}(v)$ in Fig. 3. Also plotted are an exact Maxwellian $f_{\mathrm{M}}^{(8)}(v)$ and $f_{\kappa}(v)$ for $\kappa = 8$. The particular value $N = 8$ is chosen so that the truncated Taylor expansion has the same number of poles as $f_{\mathrm{P}}(v)$, and the value $\kappa = 8$ is chosen so that the kappa distribution has the same behaviour as the truncated Taylor expansion for large values of v. As can be seen from Fig. 3, the four different distribution functions are very similar in overall shape.

Comparing the distributions in Fig. 3, we find that the truncated Taylor expansion is generally better than the kappa distribution in approximating the Maxwellian. For large v, these two functions behave like $1/v^{2N}$, and thus are better approximations to the Maxwellian than $f_{\mathrm{P}}(v)$, for which only the zeroth-

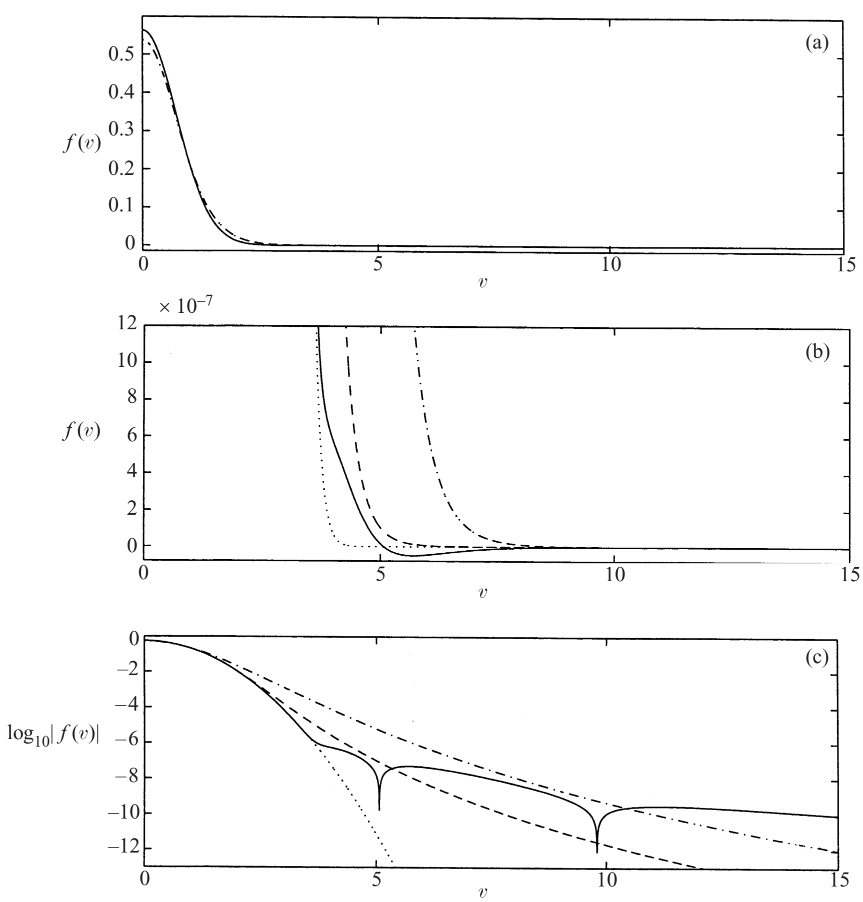

Figure 3. A comparison between four different distribution functions: ·········, the true Maxwellian distribution function as in (1.1); ———, the distribution function $f_P(v)$, from (3.4) and Table 1, implicitly used by Rönnmark (1982); ----, the truncated inverted Taylor expansion of the Maxwellian $f_M^{(N)}(v)$, from (4.2) used by Löfgren and Gunell (1997), for $N = 8$; ·–·–·–, the one-dimensional kappa distribution (Summers and Thorne 1991), from (4.4) with $\kappa = 8$. (a) Linear scale. No major differences are visible. (b) Magnification of part of (a). (c) Logarithmic plot of the magnitude of the distributions, where zeros show as negative spikes.

order moment converges. However, for $v \lesssim 4$, $f_P(v)$ is seen to follow the true Maxwellian with very good accuracy. On the other hand, $f_P(v)$ is negative for a range of values approximately between $v = 5.082$ and $v = 9.796$.

Although we do not see any immediate physical consequences of $f(v) < 0$ for a limited range of velocities, an indirect implication is that the distribution function will have positive derivative between $v = 5.707$ and $v = 11.141$, which is seen in Fig. 4. As a positive slope in the distribution function causes an instability, a calculation based on the plasma dispersion function (3.1) with coefficients as in Table 1 must lead to spurious instabilities. That such spurious or numerical instabilities indeed exist in this approach was noted already by Rönnmark (1982). By studying the difference between the imaginary parts of the Padé approximant and the plasma dispersion function, he showed that this

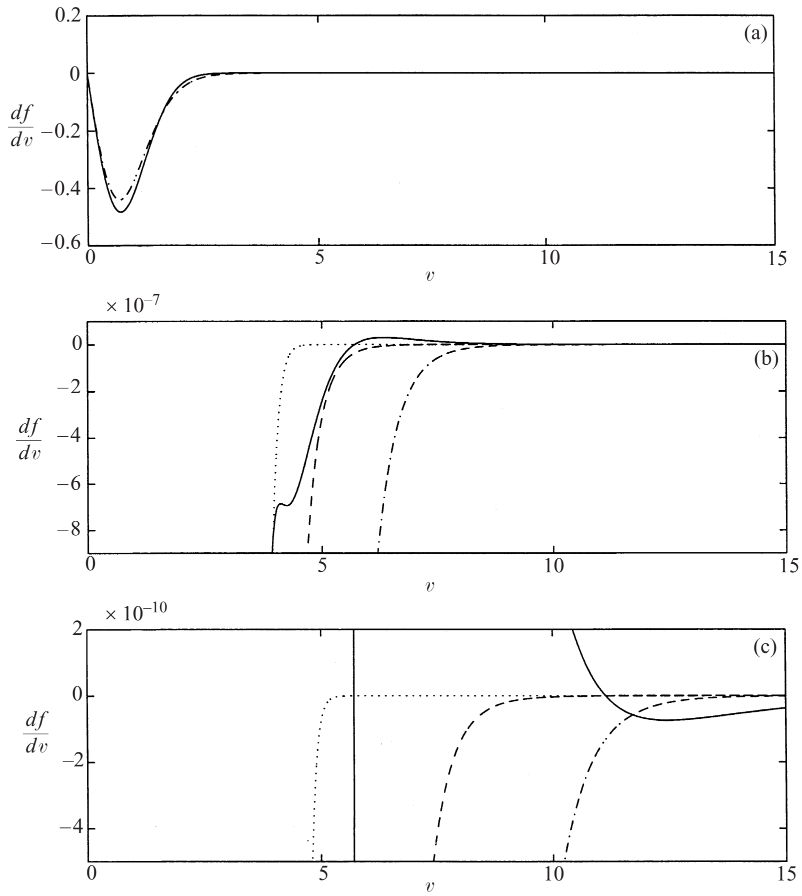

Figure 4. A comparison between the derivatives df/dv of four different distribution functions $f(v)$. The distribution functions are the same as in Fig. 3. (a) Linear scale. No difference is visible. (b) Magnification of part of (a). (c) Greater magnification of part of (a).

error generally is small and seldom significant. In our approach, we find that the imaginary part of $Z_{\mathrm{P}}(s)$ for real s can be calculated straightforwardly as

$$\operatorname{Im} Z_{\mathrm{P}}(s) = \operatorname{Im}\left(\sum_j \frac{A_j}{s-B_j}\right) = \frac{1}{2i}\sum_j \left(\frac{A_j}{s-B_j} - \frac{A_j^*}{s-B_j^*}\right). \tag{4.5}$$

If we use (3.4) we immediately find that

$$\operatorname{Im} Z_{\mathrm{P}}(s) = \pi f_{\mathrm{P}}(s). \tag{4.6}$$

This implies that the difference between $f_{\mathrm{P}}(v)$ and $f_{\mathrm{M}}(v)$ (plotted in Fig. 5) only differs from the absolute error of $\operatorname{Im} Z_{\mathrm{P}}(s)$ (plotted in Fig. 4 of Rönnmark 1982) by a factor of π.

The result that spurious instabilities appear when approximating the plasma dispersion function by the Padé approximant exist is thus not new; what is new is our physical interpretation of this behaviour in terms of the properties of the distribution function (3.4). The appearance of this numerical problem is here seen to be a natural consequence of a region of positive slope in the distribution function that is implicitly assumed.

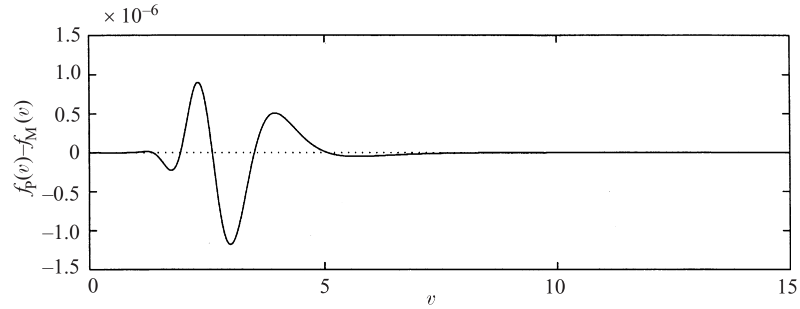

Figure 5. The difference between $f_P(v)$ and $f_M(v)$.

5. Conclusions

We have seen that the Padé approximant of a Maxwellian that is used in WHAMP corresponds to using a simple-pole distribution function to describe the plasma particles. This function is shown to be non-positive for a range of v, which implies that there is a region of positive df/dv and hence also instabilities. The result that spurious instabilities appear when approximating the plasma dispersion function by a Padé approximant is not new (see e.g. Rönnmark 1982, but what is new is our physical interpretation of this behaviour in terms of the properties of the distribution function (3.4). In our approach, this numerical problem is seen to be a natural consequence of a region of positive slope in the distribution function that is implicitly assumed.

Sometimes the problem of numerical instabilities must be avoided. An alternative may then be to use some other simple-pole approximation to the Maxwell distribution – for example the inverse of the truncated Taylor expansion (4.2). However, it should be realized that for purposes such as calculating the plasma dispersion function, the advantage of avoiding the spurious instabilities will in most cases not motivate the less accurate approximation of the Maxwellian at small velocities, and there will be little or no advantage in leaving the efficient Padé method. Whatever approximation method is used, our method of interpreting approximations of the plasma dispersion function in terms of the equivalent approximation of the particle distribution function is a powerful tool giving additional physical insight.

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