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A comparison of approximation methods for kinetic corrections to lineshape predictions

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Abstract. The present work evaluates two ways of approximating the spectral function $S(k, \omega)$ in the kinetic regime ($Kn \to 1$), by calculating the predictions of these methods for a simple model of the Boltzmann equation, and comparing those predictions with exact results. The perturbed eigenvalue approximation, used in this context for the first time, is shown to be clearly superior to the other method considered (a generalised hydrodynamic approximation), both in rapidity of convergence at fixed Kn, and in range of applicability in Kn.

1. Introduction

It is of interest to investigate the way in which the number density fluctuation spectrum $S(k, \omega)$, observed experimentally by light scattering and neutron scattering in fluids, changes from the shape predicted by hydrodynamics, as the wavelength k^{-1} becomes as small as the order of a mean free path in the fluid. For a dilute gas, one may in principle obtain $S(k, \omega)$ theoretically from the Boltzmann equation. In the hydrodynamic regime (wavenumber k small compared with an inverse mean free path), these predictions agree with those following from the equations of hydrodynamics. For k of the order of a mean free path (the kinetic regime), various approximations have been suggested for obtaining kinetic corrections to the hydrodynamic lineshape predictions. A number of these approximation methods have been reviewed by Clark (1975 and references therein), who compares a variety of lowest-order kinetic correction predictions with 'exact' results following from a 21-moment model approximation to the Boltzmann equation (see e.g. Sugawara *et al* 1968), and with experiment.

Here a simple model equation, whose properties can be found explicitly for any wavenumber k and frequency ω, is considered in place of the full Boltzmann equation. The exact spectral function $S(k, \omega)$ obtained from this model equation is compared with predictions obtained by applying two different approximation procedures (neither considered by Clark (1975)) to that same model equation, over a range of wavelengths. These comparisons should indicate how effective the same approximation procedures will be when applied to the Boltzmann equation itself. The study should be regarded as a first step towards the goal of developing a successful approximation procedure, simple to use, which can also serve as an independent check on the kinetic modelling method in at least part of the kinetic regime.

Generalised hydrodynamics (Bixon *et al* 1971, Selwyn and Oppenheim 1971) gives expressions for the Fourier–Laplace transforms of the hydrodynamic moments of the

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Boltzmann equation which are formally exact throughout the kinetic regime. To obtain physical predictions from this formalism, however, approximation is also necessary. The first approximation method considered here is one proposed by Bixon *et al* (1971) in conjunction with their formulation of generalised hydrodynamics.

The second approximation method dealt with here is related to the method for deriving kinetic corrections to sound propagation predictions originally proposed by Wang Chang and Uhlenbeck (1970). As discussed by Foch and Ford (1970), that method can be recast as a perturbed eigenvalue expansion. As shown below, the approach can be generalised in such a way as to predict kinetic corrections to lineshape predictions. One conclusion of the present study is that, while both approximation procedures are perfectly valid, the one based upon the perturbed eigenvalue expansion is clearly more successful. It not only gives closer agreement, order-for-order, than that of Bixon *et al* (1971), but it continues to be a usable procedure at values of the wavenumber k so large that the generalised hydrodynamic approximation breaks down.

2. One-dimensional model equation

The equation used here in place of the full Boltzmann equation is the one-dimensional model equation

$$\left(\frac{\partial}{\partial t}+c\frac{\partial}{\partial x}\right)h = J[h] = -(h-n) \tag{1}$$

where h is the deviation from absolute equilibrium of the number density distribution function

$$f = f^0(1+h)$$

and n is the deviation of the number density from its equilibrium value (all variables are non-dimensional, and the external length scale is a mean free path). Equation (1) describes a simple diffusive system, with the number density n as the single conserved quantity. Some of its properties have been discussed by Goebel and Johnson (1979) and a similar equation has been considered by Résibois and de Leener (1977). The lineshape predicted by equation (1) is that discussed in some detail by Nelkin and Ghatak (1964). It exhibits the well known change from simple diffusive broadening at small k to Doppler broadening at large k, and is known exactly for all k.

The structure function which results from equation (1) in the hydrodynamic regime is the Lorentzian

$$S_L(k,\omega) = \frac{2Dk^2}{\omega^2+(Dk^2)^2} \tag{2}$$

where D is the constant (non-dimensionalised) coefficient of diffusion; its value is

$$D = \tfrac{1}{2} \tag{3}$$

for this model. When k ceases to be small, kinetic corrections must be made to equation (2). As suggested by Selwyn and Oppenheim (1971), these corrections depend not only upon k, but also on ω, to lowest order.

The exact solution for $S(k, \omega)$ following from (1) is obtained by imposing the initial condition

$$h(x, c, t=0) = \sqrt{2\pi}\delta(x) \tag{4}$$

and using the definition

$$S(k, \omega) = 2 \operatorname{Re} n(k, \omega + i\delta) \qquad \begin{pmatrix} \delta \to 0^+ \\ k, \omega \text{ real} \end{pmatrix} \tag{5}$$

where $n(k, \omega)$ is the Fourier–Laplace transform of the number density

$$n(x, t) = \langle 0 | h(x, t) \rangle$$

(a summary of notation and mathematical properties is contained in the appendix). The exact solution for $n(k, \omega)$ following from (1) is

$$n(k, \omega) = [-i\omega + ik(Z^{-1} + z)]^{-1} \tag{6}$$

where $Z(z)$ is the plasma dispersion function (Fried and Conte 1961)

$$Z(z) = \int_{-\infty}^{\infty} \frac{e^{-c^2}}{\sqrt{\pi}} \frac{dc}{c - z} \tag{7}$$

and

$$z \equiv x + iy = \left(\frac{\omega}{k} + \frac{i}{k}\right). \tag{8}$$

Z is a tabulated function (Faddeyeva and Terent'ev 1961).

3. A generalised hydrodynamic approximation

The generalised hydrodynamic approach of Bixon *et al* (1971) will be considered in detail here, combined with the approximation procedure suggested by those authors, and applied to derive the lineshape resulting from the model equation (1). (Some other aspects of generalised hydrodynamics, as applied to one-dimensional model equations, have been discussed by Goebel and Johnson (1979).)

From the results of Bixon *et al* (1971), using the notation of the appendix herein, all collisional contributions to the Fourier–Laplace transformed equations for the hydrodynamic moments of the Boltzmann (or model) equation are contained in the matrix elements

$$D_{\alpha\beta} = \langle \alpha | P(-i\omega + PLP)^{-1} P | \beta \rangle \tag{9}$$

where L is the operator

$$L = i\boldsymbol{k} \cdot \boldsymbol{c} - \varepsilon^{-1} J, \tag{10}$$

ε is a scale factor set equal to unity in the present work, and J is the linearised Boltzmann (or model) collision operator. P is the projection operator onto the space of all those states orthogonal to the hydrodynamic states. As discussed by Goebel and Johnson (1979), equation (1) describes a system with a single hydrodynamic state $|0\rangle$, and a single generalised hydrodynamic equation. For the given initial condition (4), this

equation becomes

$$(-\mathrm{i}\omega - \tfrac{1}{2}kD_{11})n(k,\omega) = 1 \tag{11}$$

where D_{11} can be obtained analytically, giving the Nelkin–Ghatak profile (6) for $S(k,\omega)$.

In order to test the approximation procedure suggested by Bixon *et al* (1971), one approximates the matrix element (9) using the operator identity

$$(-\mathrm{i}\omega + PLP)^{-1} = (-\mathrm{i}\omega - J/\varepsilon)^{-1} - (-\mathrm{i}\omega - J/\varepsilon)^{-1} P\, \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{c}P(-\mathrm{i}\omega + PLP)^{-1}. \tag{12}$$

This gives the matrix elements $D_{\alpha\beta}$ in terms of the (presumably more familiar) matrix elements of the operator $(-\mathrm{i}\omega - J/\varepsilon)^{-1}$. As noted by Goebel and Johnson (1979), the expansion (12) gives D_{11} as a power series in z^{-2n}, where z is defined by equation (8), yielding

$$S(k,\omega) = 2\,\mathrm{Re}\,\mathrm{i}\left[\omega - k\left(\frac{1}{2z} + \frac{1}{2z^3} + \frac{5}{4z^5} + \frac{37}{8z^7} + \ldots\right)\right]^{-1}. \tag{13}$$

When $k \to 0$, equation (13) reduces to the Navier–Stokes prediction of equation (2).

4. Perturbation approximation

To use the perturbed eigenvalue expansion discussed by Foch and Ford (1970) for predicting kinetic corrections to lineshape predictions, one may write the Fourier–Laplace transform of equation (1) in the form

$$(J + \lambda c)h = Eh - 1 \tag{14}$$

with the use of initial condition (4), where

$$E = -\mathrm{i}\omega, \qquad \lambda = -\mathrm{i}k. \tag{15}$$

Here $h = h(k,\omega)$ is the transform of $h(x,t)$. One then generates an approximate solution by writing

$$\begin{aligned} E &= E_0 + \lambda E_1 + \lambda^2 E_2 + \ldots \\ h &= h_0 + \lambda h_1 + \lambda^2 h_2 + \ldots \end{aligned} \tag{16}$$

and equating like powers of λ. Uniqueness is obtained by demanding that h_0 has non-zero overlap with $n(k,\omega)$ and is orthogonal to all higher-order corrections:

$$\langle h_0 | h_i \rangle = 0, \qquad i \neq 0. \tag{17}$$

One obtains for

$$n(k,\omega) = \langle 0 | h(k,\omega) \rangle \equiv A_0 \tag{18}$$

the equation

$$A_0[-P - (E_0 + \lambda E_1 + \ldots) + \lambda c](h_0 + \lambda h_1 + \ldots) + (1-P)(h_0 + \lambda h_1 + \ldots) = 0. \tag{19}$$

By equating successively higher powers of λ, one generates expressions for successive

terms in E_0 and h_i, in terms of the moment $n = A_0$. Thus,

$$\begin{aligned} &E_0 = A_0^{-1}, && |h_0\rangle = |0\rangle A_0; \\ &E_1 = 0, && |h_1\rangle = |1\rangle A_1^{(1)}; \\ &A_1^{(1)} \equiv \langle 1|h_1\rangle = \frac{\Omega_{10} A_0}{(1 + A_0^{-1})}; \end{aligned} \tag{20}$$

$$\ldots$$

($\Omega_{\alpha\beta}$ is the kinematic coupling matrix defined in equation (A7). On the other hand, if one takes the $\langle 0|$ moment of the transform equation (14), one obtains the continuity equation

$$En(k, \omega) + \mathrm{i}ku(k, \omega) = 1 \tag{21}$$

where

$$\sqrt{2}u = \langle 1|h\rangle \equiv A_1. \tag{22}$$

The successive approximations given by equation (19) generate an expansion for the moment A_1:

$$A_1 = \sum_{m=0} \lambda^m A_1^{(m)} \equiv \sum_{m=0} \lambda^m \langle 1|h_m\rangle \tag{23}$$

which is of the form

$$A_1^{(2m+1)} \propto A_0 (1 + A_0^{-1})^{-(2m+1)}.$$

Using equation (21), one thus obtains

$$n(k, \omega) = A_0 = \mathrm{i}\left[\omega - k \sum_{m=0} C_{2m+1} \left(\frac{-\mathrm{i}k}{1 + A_0^{-1}}\right)^{2m+1}\right]^{-1} \tag{24}$$

where explicit values for the C_i are found to be

$$C_1 = \tfrac{1}{2} \qquad C_3 = \tfrac{1}{4} \qquad C_5 = \tfrac{1}{2} \ldots . \tag{25}$$

To each order m of approximation, equation (24) gives an implicit expression for the mth approximation to $n(k, \omega)$. The solution of the full implicit equation (24) will be taken to *define* the perturbed eigenvalue mth approximation to $n(k, \omega)$.

Instead of solving the full equation (24), one could use an iterative re-approximation, treating A_0^{-1} as a small parameter on the right-hand side of equation (24), and obtaining $A_0^{(m)}$ explicitly in terms of $A_0^{(m-1)}$. Direct solution of the full implicit equation (24), however, was found to give much better agreement with exact results. (For instance, the iterative re-approximation to equation (24), to lowest order, gives the Lorentzian lineshape (2) predicted by hydrodynamics, whereas the exact lowest-order approximation

$$2A_0^{-1} = -(1 + \mathrm{i}\omega) + [1 + 2k^2 - \omega^2 - 2\mathrm{i}\omega]^{1/2} \tag{26}$$

agrees with the Lorentzian prediction (2) for small k, but continues to give surprisingly good lineshape predictions well into the kinetic regime.)

5. Effectiveness of approximation procedures

Both the generalised hydrodynamic procedure (BDM) and the perturbation (P) procedure give good approximations to the lineshape for small k. A comparison of maximum errors, for several orders of approximation, is given in table 1 for 'large' y ($= 10, 5, 3$), where $y = k^{-1}$ is the ratio of wavelength to mean free path. Here BDM(m) refers to the approximation resulting from equation (14) when terms to order z^{2m+1} are retained, while P(m) refers to the perturbation approximation given by equation (24) when terms to order m are retained. The relative percentage error Δ is, by definition, the maximum value of

$$|S_i/S_{\text{exact}} - 1| \times 100$$

in the frequency range considered, $\omega \leqslant 1.5k^2$, which contains the main contribution to $S(k, \omega)$.

Table 1. Kinetic corrections for large y.

	Relative error (%)		
y	10	5	3
Lorentzian	1	4	8.9
BDM(0)	1	4	8.9
BDM(1)	10^{-2}	0.4	2.5
BDM(2)	10^{-4}	0.05	0.9
P(0)	0.5	2	4.1
P(1)	10^{-2}	0.1	0.8

As expected, the accuracy of both procedures decreases with decreasing y. For large y, both approximation methods work well, the perturbation approximation giving somewhat better predictions, order-for-order. As y decreases the perturbation approximation becomes increasingly better, in comparison with BDM, so that for $y = 3$, the first-order perturbation approximation already gives better predictions than the second-order BDM approximation.

As y decreases, the difference between the predictions of the two methods increases. Figure 1 shows the first three BDM approximations plotted against the exact lineshape for $y = 2$; the slow convergence is evident. A similar plot for the first two perturbation approximations is given in figure 2, and the relative (percentage) errors for both methods are plotted in figure 3. The advantage of the perturbation approach is evident here. By the time $y = 1.5$, the BDM method cannot be used because its errors increase as higher-order approximations are used. The perturbation method is still a useful approximation scheme, however, although convergence has become slower.

For $y = 1$ (wavelength equal to a mean free path), neither method is a useful approximation scheme. The lowest-order perturbation prediction for the lineshape, however, continues to follow the exact lineshape better than might have been expected (errors for $y = 1.5$ and $y = 1.0$ are shown in figure 4) and even in the extreme case $y = 0.02$, its peak height prediction is only about 20% too low.

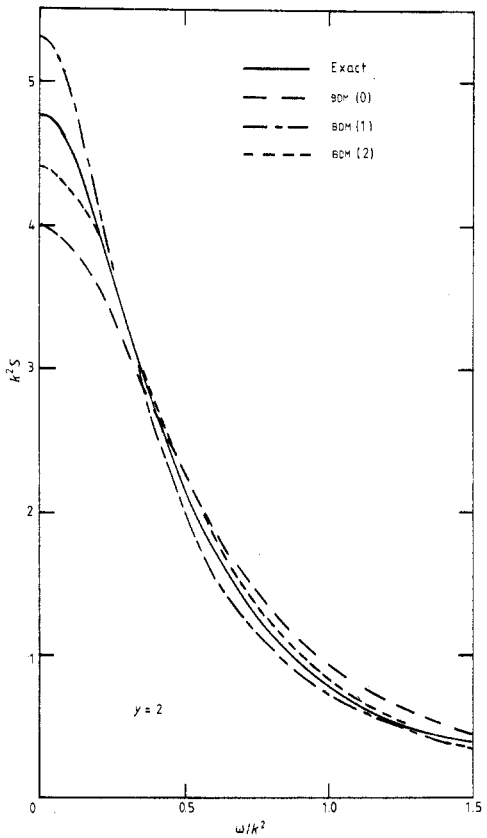

Figure 1. BDM lineshape approximations $m = 0$, 1, 2, and exact lineshape, $y = 2$.

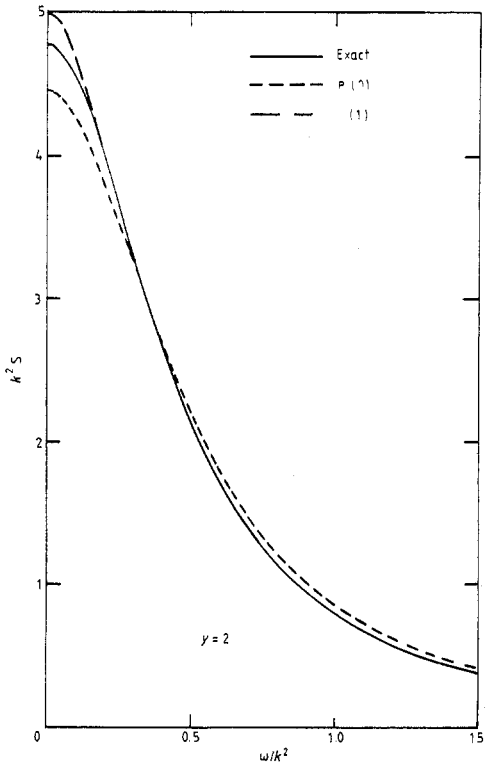

Figure 2. P approximations $m = 0$, 1, and exact lineshape, $y = 2$.

6. Discussion

The present study compares several lineshape approximations in the kinetic regime with exact results, for a model gas. Clark (1975) compares the results of various other approximations, taken to lowest order, with 'exact' 21-moment kinetic modelling predictions for Maxwell and hard sphere gases. Although there is no point of direct comparison, several general points may be made. One of Clark's conclusions is that the generalised hydrodynamic approximation of Selwyn and Oppenheim (1971) gives better agreement with 21-moment kinetic modelling predictions, for a Maxwell gas, (and thus with experiment) than the Burnett approximation of Ranganathan and Nelkin (1967). From Clark (1975) one sees that the maximum deviations of the former from 'exact' results are about 4%, and of the latter about 6% for $y \geqslant 3$. Here, at the same values of y, the generalised hydrodynamic approximation BDM(1) deviates from exact results by at most 2.5%, while the perturbation approximation P(1) shows a maximum deviation of only 0.8%.

Clark (1975) also presents 'Selwyn approximate' predictions, which seem to reproduce the shape of the central peak with roughly the same accuracy and range of applicability as the present P(0) prediction does, at least for $y > 1$.

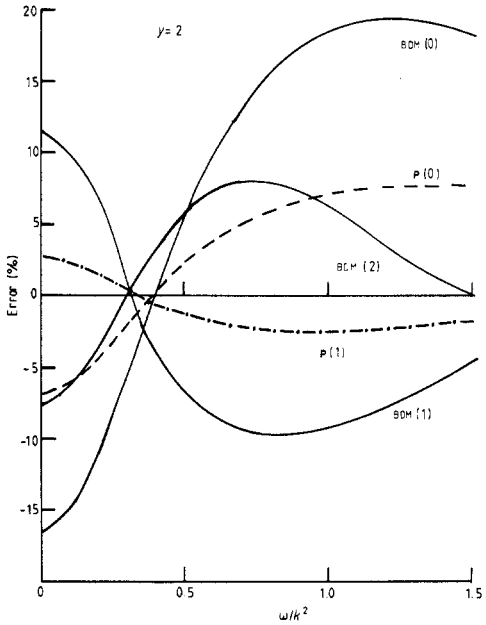

Figure 3. Error (%) of Bixon *et al* (1971) (BDM) and perturbation (P) lineshape approximations, relative to exact result, $y = 2$.

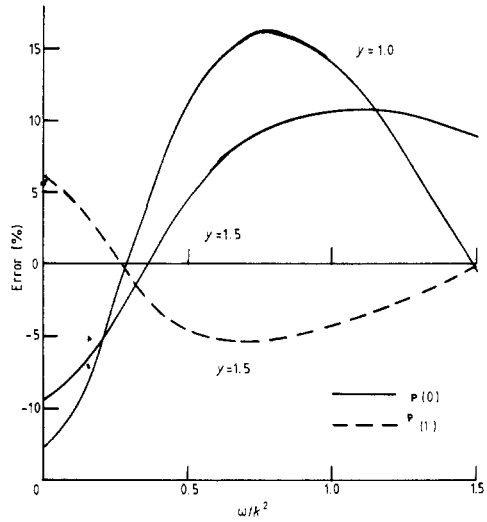

Figure 4. Error of P lineshape approximations, relative to exact result, $y = 1.5$ and $y = 1.0$.

7. Concluding remarks

The perturbed eigenvalue approximation for lineshapes has been used here with a simple model of the Boltzmann equation. Its extension to the full Boltzmann equation proceeds similarly and is straightforward (but more complicated), at least for a gas of Maxwell molecules. In view of the present success of the method, it would seem worthwhile to carry out an investigation similar to that of Clark (1975) for evaluating the perturbed eigenvalue lineshape approximation for the full Boltzmann equation. If, as seems possible, the method gives good results because of the mathematical structure of the approximation (in a similar way to, say, a Padé approximant or continued fraction approximation), then one might expect this method also to be advantageous for the full Boltzmann equation as it is for the present model equation.

The generalised hydrodynamic approximation procedure considered here is, nevertheless, a valid way of obtaining kinetic corrections to lineshape predictions. The implication of the present study is not that the generalised hydrodynamics of Bixon *et al* (1971) has failed, but rather that better approximation procedures than that originally suggested by Bixon *et al* (1971) are needed in the context of their exact formalism.

Finally, one may remark that the perturbed eigenvalue approach outlined in Foch and Ford (1970) may properly be thought of as another kind of 'generalised hydrodynamics', albeit an intrinsically approximate one.

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Appendix. One-dimensional model gases—notation and properties

One may expand the perturbation h to the number density distribution function in a complete orthonormal set of states $|\alpha\rangle$:

$$|h\rangle = |\alpha\rangle A_\alpha \tag{A1}$$

where $\langle\alpha|\beta\rangle = \delta_{\alpha\beta}$, and sum over α is implied. The moments of h are

$$A_\alpha \equiv \langle\alpha|h\rangle = \int_{-\infty}^{\infty} dc\, w(c)\phi_\alpha(c)h(c) \tag{A2}$$

with respect to the weight function

$$w(c) = e^{-c^2}/\pi^{1/2}, \tag{A3}$$

and it is convenient to choose the expansion functions to be

$$\phi_\alpha(c) \equiv \langle c|\alpha\rangle = H_\alpha/(2^\alpha \alpha!)^{1/2}, \tag{A4}$$

where H_α are the Hermite polynomials

$$H_\alpha = (-1)^\alpha e^{c^2} \frac{d^\alpha (e^{-c^2})}{dc^\alpha}; \tag{A5}$$

these are the one-dimensional analogues of the Burnett functions. The first few moments of h are then

$$A_0 = \langle 0|h\rangle = n, \qquad A_1 = \langle 1|h\rangle = \sqrt{2}u, \qquad A_2 = \langle 2|h\rangle = E/\sqrt{2}, \tag{A6}$$

where n, u and E are the deviations from equilibrium of the number density, flow velocity and energy density, non-dimensionalised with respect to equilibrium parameters in density ρ_0 and pressure p_0, and to the reference velocity $(2p_0/\rho_0)^{1/2}$. The kinematic coupling matrices

$$\Omega_{\alpha\beta} \equiv \langle\alpha|c|\beta\rangle \tag{A7}$$

in one dimension have the values

$$\Omega_{\alpha,\alpha+1} = \Omega_{\alpha+1,\alpha} = [(\alpha+1)/2]^{1/2}; \qquad \Omega_{\alpha,\beta} = 0, \qquad \beta \neq \alpha \pm 1. \tag{A8}$$

One may write a class of simple model equations in the form

$$\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)|h\rangle = -\varepsilon^{-1} P|h\rangle \tag{A9}$$

where P is the projection operator

$$P = 1 - |\sigma\rangle\langle\sigma| \tag{A10}$$

and the states $|\sigma\rangle$ are the 'hydrodynamic states', i.e. those chosen to represent conserved quantities. Different aspects of the linearised Boltzmann equation are modelled by different choices for the set $\{\sigma\}$.

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