Evolution of density discontinuity in rarefied plasma kinetics

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A study is made of the motion of a rarefied plasma as a result of decay of a density discontinuity. Plasma is described by a kinetic equation with a self-consistent field which is solved numerically by the particle-in-cell technique. It is shown that eventually the motion approaches the self-similar solution considered by Gurevich, Pariĭskaya, and Pitaevskiĭ [Sov. Phys. JETP **22**, 449 (1966); **27**, 476 (1968); **36**, 274 (1973)]. It is shown that the self-similar solution describes correctly the acceleration of ions in a plasma expanding in vacuum.

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§1. INTRODUCTION

The flow of a continuous medium due to decay of a discontinuity has been investigated in detail in gasdynamics[1] and gaskinetics.[2,3] In particular, it is known that under certain conditions this flow can have scaling similarity and can be described by self-similar (scaling-invariant) solutions of the appropriate equations. The problem of decay of a discontinuity is more complex in the kinetics of a rarefied plasma. Gurevich *et al.*[4] have shown that there is a limiting self-similar motion of a plasma which is attained when the characteristic spatial scale of the motion becomes much greater than the Debye radius and appropriate solutions of the kinetic equation with a self-consistent field are obtained.

However, there has been no systematic study of the attainment of this self-similar limiting regime by a flow originating from an initial discontinuity. This is of interest because of the numerous applications of the solutions found by Gurevich *et al.*[4] in the analysis of problems in ionospheric aerodynamics and laser plasma dynamics, which are of practical importance. One of the typical examples is the problem of ion acceleration in an expanding plasma. It follows from the results of Gurevich *et al.*[4,5] that expansion of a plasma in vacuum is accompanied by acceleration of a considerable proportion of the total number of ions to energies considerably greater than the average thermal value. In the case of a multicomponent plasma the energy of such accelerated ions is approximately proportional to their charge,[5] which is in agreement with the experimental results (see Ref. 6 and the references given there).

The question of ion acceleration was considered also by Widner *et al.*[7] and by Mulser.[8] Numerical calculations carried out using the hydrodynamic model yielded a certain limiting ion velocity, approximately equal to three times the average thermal velocity.[7] Mulser[8] used similar hydrodynamic calculations to conclude that the maximum energy of the accelerated ions is independent of their charge. These conclusions were very different from the results of Gurevich *et al.*[4,5]

Clearly, the hydrodynamic approximation is fairly rough when applied to the problem of expansion of a plasma in vacuum; the kinetic formulation of the problem adopted by Gurevich *et al.*[4,5] is more correct.[1)]

However, the quantitative results of Gurevich *et al.*[4,5] on the accelerated group of ions had to be refined somewhat because the self-similar solution is not valid throughout the space-time domain in which the ion acceleration takes place.

It thus becomes necessary to solve the general self-similar problem of the motion of a plasma created by a density discontinuity. We shall tackle this problem by numerical methods. The solution obtained will be compared with the self-similar solution[4,5] and the range of validity of the latter will be found. Calculations will be reported for a two-component plasma with various ratios of the masses of the components and also for the model of a plasma with a local equilibrium distribution of electrons used by Gurevich *et al.*[4,5] The question of ion acceleration in one- and two-temperature plasmas will be considered in detail.

We shall use the particle-in-cell method[9] to solve the collisionless kinetic equation. The methodological features of the variant of the method used are described elsewhere.[10] A comparison of the self-similar solution with the exact one requires more detailed information on the distribution of the variables than that which can be obtained from the graphs of Gurevich *et al.* (Refs. 4 and 5).[2)] Consequently, we prepared a special program for the solution of the self-similar problem and used it to carry out detailed calculations of the ion distribution function in a wide range of plasma parameters. The solution method was similar to that used by Gurevich *et al.*[4,5] but we were able to avoid the incorrect operation of numerical differentiation.

The results for the same variants are in good agreement with those of Gurevich *et al.*[4,5] By way of example, Fig. 1 shows two families of integral curves of the self-similar solution in the plane of the two variables

$$u=v(m_i/2T_e)^{1/2},\quad \tau=(x/t)(m_i/2T_e)^{1/2};$$

the curves correspond to the values of the ratio $\beta = T_e/T_i = 1$ and $\beta = 10$. The principal properties of the self-similar solution follow readily from Fig. 1: an increase in τ results in unbounded acceleration of ions and a

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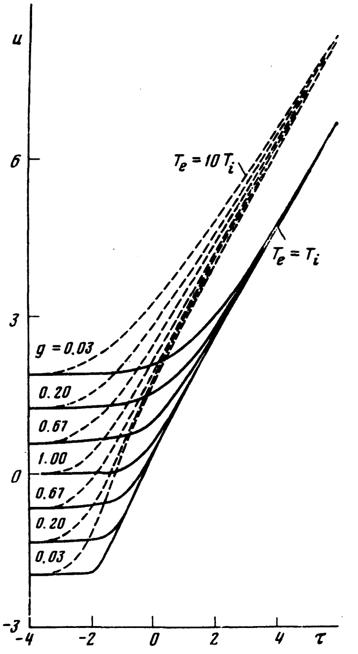

FIG. 1. Characteristics of the self-similar solution in the $u\tau$ plane. The continuous curves correspond to $\beta = 1$ and the dashed curves to $\beta = 10$; g represents the ion distribution function.

simultaneous reduction in their temperature (the distribution function tends to a delta-like shape); the acceleration of ions increases with the initial electron temperature.

§2. STRUCTURE OF FLOW. COMPARISON WITH SELF-SIMILAR SOLUTION

Decay of a density discontinuity begins with the motion of the electron component; the electric field resulting from the charge separation is responsible for the ion acceleration. The process of ion acceleration then continues and at the same time the total energy of the electron component decreases when the ion increases. The distribution of the electric field at various moments is shown in Fig. 2b. This figure gives the results of calculations carried out on the assumption that electrons have a local equilibrium distribution function in a self-consistent field corresponding to an instantaneous distribution of the charge density (formally, this case corresponds to the mass ratio $m_i/m_e \to \infty$). Initially, a narrow peak of the field intensity appears in the vicinity of a discontinuity and this peak eventually expands and decreases in amplitude. The time (in units of ω_{pi}^{-1}) is given alongside each curve. For comparison, this figure includes the field distributions calculated for the same moments from the self-similar solution.[4] The points on the continuous curves show the successive positions of the boundary of an expanding ion cloud. We can see that a considerable difference between the self-similar and exact field profiles appears only in the region ahead of the ion front, where the conditions of validity of the self-similar solution are not satisfied.

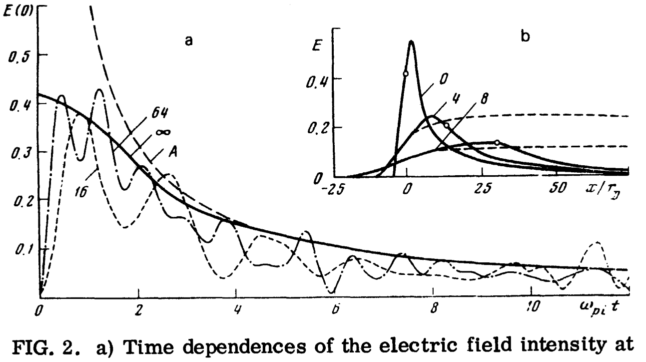

FIG. 2. a) Time dependences of the electric field intensity at the point $x = 0$. The curves differ in respect of the ion mass. A represents the self-similar solution. b) Spatial distribution of the electric field at various moments. The dashed curves give the self-similar solution. The points on the continuous curves are the positions of the ion front.

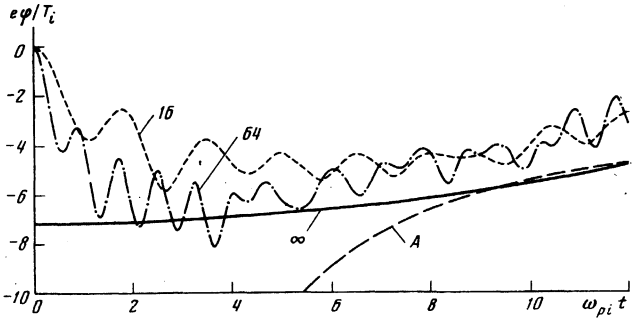

FIG. 3. Potential at the point $x/r_D = 50$ plotted as a function of time for various values of the ratio m_i/m_e; A is the self-similar solution.

Figure 2a gives the time dependence of the electric field at the point of the initial density discontinuity $x = 0$. The dashed curve represents the self-similar solution and the other curves found by numerical solution for various values of the mass ratio $\mu = m_i/m_e$. Considerable differences between the curves are observed only during the initial stage of the expansion.

In the case of finite mass ratios ($\mu = 16,\ 64$) the intensity (Fig. 2a) and the potential (Fig. 3) of a self-consistent electric field oscillate with time. These oscillations, like those discussed earlier,[10] make it difficult to compare the numerical and self-similar solutions so that we shall make this comparison employing the results of calculation for a model with local equilibrium electrons. The corresponding profiles of the potential φ (in units of T_i/e) are shown for various moments in Fig. 4. The dashed lines in this figure

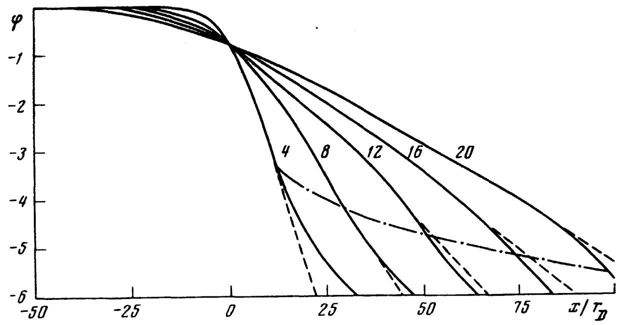

FIG. 4. Potential plotted as a function of the variable x/r_D at various moments in time. The chain curve is the position of the ion front.

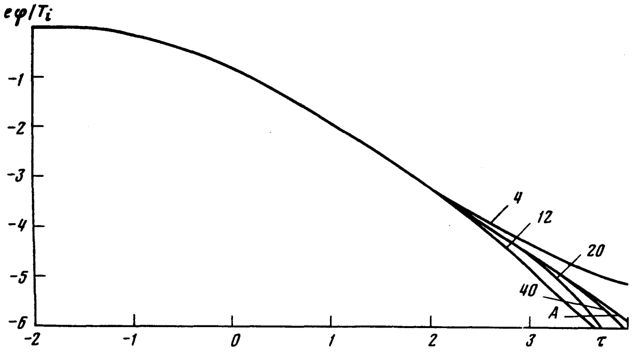

FIG. 5. Potential plotted as a function of the self-similar variable τ at various moments in time. The self-similar solution is curve A.

represent the self-similar solutions; the chain line intersecting all the curves is the position of the ion front. It follows from Fig. 4 that throughout most of the region where the ion density does not vanish, the self-similar solution is very close to the exact one. Some difference between the potential profiles are observed only near the moving ion front where the quasi-neutrality condition is not satisfied.

It is interesting to note that, in contrast to many problems in which the solution evolves with time in such a way as to approach monotonically the asymptotic self-similar result, in the present case the attainment of the self-similar regime is nonmonotonic: the difference between the exact and self-similar values of the potential in the vicinity of the ion front oscillates with time. This is shown particularly clearly in Fig. 5, which gives the dependence of the potential on the self-similar variable τ at various moments in time (the values of $\omega_{pi}t$ are given alongside each curve; A is the self-similar solution). It is clear from Fig. 5 that eventually the self-similar profile of the potential is established throughout a wide range of the variable τ. The boundary of the region where the self-similar solution applies is close to the ion front ahead of which the deviation of the profile from the self-similar solution alternates from positive to negative values.

It is clear from our results that the self-similar solution gives a correct asymptotic description of the flow resulting from a density discontinuity. The self-similar solution is inapplicable during the initial stage of the discontinuity decay and in the vicinity of an ion front. It also does not describe the oscillations of the electric field at frequencies of the order of the electron plasma value, which appear if allowance is made for the finite electron mass.

§3. ION ACCELERATION

An analysis based on the self-similar solution[5] indicates that expansion of a plasma in vacuum results in the acquisition by a considerable proportion of ions of an energy which is many times greater than the average thermal value. Ion acceleration occurs as a result of the action of an electric field. Since the distribution of the field intensity given by the self-similar solution differs slightly from the exact one (Fig. 2b), it is interesting to study the influence of this difference on the distribution function of accelerated ions. The fullest information on the particle acceleration can be obtained by determining the local distribution function. However, in the particle-in-cell method such a calculation presents familiar difficulties because the total number of large particles is limited. The average distribution functions in some spatial region can be calculated much more simply and more accurately. Computation of such average values for the exact self-similar solutions makes it possible to determine the range of validity of the self-similar solution in describing the motion of an accelerated group of ions.

The results given below were obtained as follows. A numerical solution at some moment t was used to calculate the average distribution functions of ions in an interval Δx selected in such a way that the corresponding interval of variation of the self-similar variable

$$\Delta\tau=\frac{\Delta x}{t}\left(\frac{m_i}{2T_e}\right)^{1/2}$$

was unity. The results of these calculations are represented by the continuous curves in Fig. 6. Next, the self-similar solution was used to find the averages of the distribution functions over several intervals of the variable τ of length $\Delta\tau = 1$ (dashed curves in Fig. 6). The parameter of this family of curves was the variable τ at the midpoint of each of the integration intervals. For convenience, the values of the average distribution functions at their maxima were taken to be unity. A comparison of the curves showed that the self-similar solution differed little from the exact one.

It should be noted that the proportion of particles with velocities six times greater than the thermal value is found to be several orders of magnitude greater than for the Maxwellian distribution, i.e., ions are indeed accelerated strongly. We should bear in mind that the quantitative results of our calculations can be affected, in a certain range of the initial plasma parameters, by the collisional effects ignored in the self-consistent field approximation. Numerical simulation of the acceleration in this range of initial densities and temperatures can be made conveniently employing a method proposed by Ivanov and Shvets.[12] The results of these calculations will be presented in a separate communication.

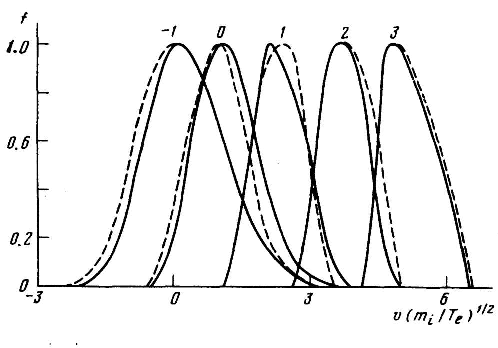

FIG. 6. Average distribution functions of ions at $\omega_{pi}t = 60$. The numbers alongside the curves are the values of τ at the midpoint of the integration interval.

The distribution function shown in Fig. 6 applies at a moment $t = 60\omega_{pi}^{-1}$. In fact, it does not change greatly beginning from $t = 10\omega_{pi}^{-1}$. A later moment is chosen solely because for a fixed value of $\Delta\tau$ the segment Δx increases proportionally with time and integration of the distribution function is carried out over this segment; this means that the number of large particles within this segment also increases proportionally to time. Consequently, the precision of the calculation of the distribution function is improved. An analysis of the results of this numerical simulation shows that, with the exception of the initial moments, the number density of large particles $\Delta N/\Delta x$ in given segments of $\Delta\tau$ remains quite accurately constant, i.e., ΔN increases linearly with time as expected for self-similar motion. Numerical values of the densities in the exact and self-similar solutions are in good agreement in a fairly wide range of the variable τ. Thus, the self-similar solution[4,5] describes correctly the dynamics of ion acceleration during expansion of a plasma in vacuum.

§4. TWO-TEMPERATURE PLASMA

If the temperatures of electrons and ions are different, the qualitative picture of the evolution of a density discontinuity remains basically the same as in the one-temperature case. However, there are important quantitative differences. It is shown in Fig. 7 how the density of ions increases at a point separated by $50r_D$ from the initial boundary of a plasma cloud for different values of the ratio $\beta = T_e/T_i$. As β increases, the rate of filling of vacuum with the plasma rises and the values of the ion density found by numerical simulation exceed somewhat the values deduced from the self-similar solution (the dashed curves in Fig. 7 correspond to the asymptote of the self-similar solution[4] in the $\beta \gg 1$ case).

The change in the electron temperature has a considerable influence on the self-consistent field potential. It follows from the self-similar solution that at the point of the initial discontinuity $x = 0$ the potential rises linearly in the absolute sense on increase of T_e/T_i. This result follows also from the numerical calculations. The values of the potential and ion density at $x = 0$ remain unchanged after a short initial period.

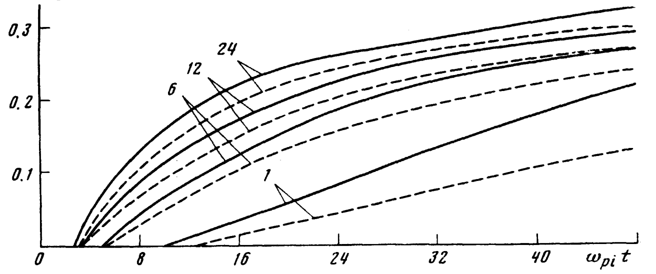

FIG. 7. Time dependences of the ion density at the point $x/r_D = 50$ for various values of β.

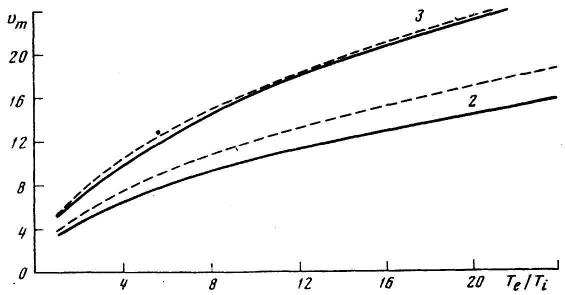

FIG. 8. Position of the maximum of the distribution function plotted as a function of the ratio T_e/T_i. The numbers alongside the curves are the values of the self-similar variable τ. The dashed curves give the self-similar solution.

An increase in the electron temperature has a strong influence on ion acceleration. In particular, the positions of the maxima v_m of the distribution functions calculated by the method described in the preceding section are shifted, on increase of T_e/T_i, toward higher velocities. The results of calculations of v_m are presented in Fig. 8. The continuous curves deduced from the numerical solution represent positions of the maxima of the distribution function integrated over the coordinate. The integration intervals Δx correspond to the segments $\Delta\tau = 1$ centered at the points $\tau = 2$ and $\tau = 3$. The dashed curves are the maxima of the local distribution functions with the same values of τ which are calculated from the self-similar solution[4,5] in the limiting case of $\beta \gg 1$. The differences between the curves are slight and are partly due to the fact that integration of the distribution function with respect to τ shifts the position of the maximum toward lower velocities. Thus, the laws governing ion acceleration in a two-temperature plasma are also described satisfactorily by the self-similar dependences deduced by Gurevich *et al.*[4,5]

The authors are deeply grateful to L. P. Pitaevskiĭ for numerous valuable discussions.

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[1] The hydrodynamic description of expansion of a neutral gas in vacuum has been considered by Anisimov and Rakhmatulina.[3]

[2] This obviously explains the fact that the self-similar solution is compared with the exact numerical solution only by Alikhanov *et al.*[11] in the limiting case of cold ions when the self-similar solution can be presented in an analytic form.

[1]L. D. Landau and E. M. Lifshitz, Mekhanika sploshnykh sred, Gostekhizdat, M., 1953 (Fluid Mechanics, Pergamon Press, London, 1959).
[2]C. K. Chu, Phys. Fluids **8**, 12 (1965).
[3]S. I. Anisimov and A. Kh. Rakhmatulina, Zh. Eksp. Teor. Fiz. **64**, 869 (1973) [Sov. Phys. JETP **37**, 441 (1973)].
[4]A. V. Gurevich, L. V. Parĭskaya, and L. P. Pitaevskiĭ, Zh. Eksp. Teor. Fiz. **63**, 516 (1972) [Sov. Phys. JETP **36**, 274 (1973)].
[5]A. V. Gurevich, L. V. Parĭskaya, and L. P. Pitaevskiĭ, Zh. Eksp. Teor. Fiz. **63**, 516 (1972) [Sov. Phys. JETP **36**, 274 (1973)].
[6]J. F. Ready, Effects of High Power Laser Radiation, Academic Press, New York, 1971 (Russ. Transl., Mir, M., 1974).

[7]M. Widner, I. Alexeff, and W. D. Jones, Phys. Fluids 14, 795 (1971).
[8]P. Mulser, Plasma Phys. 13, 1007 (1971).
[9]R. L. Morse, in: Methods in Computational Physics, Vol. 9, Plasma Physics (ed. by B. Alder, S. Fernbach, and M. Rotenberg), Academic Press, New York, 1970, p. 213 (Russ. Transl., Mir, M., 1974).
[10]S. I. Anisimov and Yu. V. Medvedev, Preprint, Landau Institute of Theoretical Physics, Academy of Sciences of the USSR, Chernogolovka, 1977.
[11]S. G. Alikhanov, V. G. Belan, G. N. Kichigin, and P. Z. Chebotaev, Zh. Eksp. Teor. Fiz. 59, 1961 (1970) [Sov. Phys. JETP 32, 1061 (1971)].
[12]M. F. Ivanov and V. F. Shvets, Dokl. Akad. Nauk SSSR 238, 1324 (1978) [Sov. Phys. Dokl. 23, 130 (1978)].

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Establishment of the vibrational distribution of diatomic molecules

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An analytic theory is developed of the establishment of the vibrational distribution function of diatomic anharmonic molecules. The solutions obtained are compared with the results of accurate numerical calculations. The rate of heating of a gas is found after the beginning of pumping and in the case of pulsed excitation of the vibrations.

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An interesting example of a system far from the equilibrium is a vibrationally excited gas of diatomic molecules. For many such molecules (for example, N_2, CO, HCl, H_2, etc.) the relaxation time τ_{V-T} of the conversion of the vibrational to the translational energy is long compared with the time taken to establish the vibrational distribution function (τ_{V-V}). This means that it is quite easy to establish a state in which a gas has low translational and rotational temperatures but is highly excited in the vibrational sense. Such a state has a number of special features which affect, for example, the dispersion of sound, the degree of dissociation of molecules, the relaxation of the vibrational energy into heat, and the possibility of a population inversion between neighboring vibrational-rotational levels (for a review see, for example, Ref. 1).

It is shown in Ref. 2 that, in the absence of the $V-T$ relaxation, the vibrational distribution of molecules is affected greatly by their anharmonicity. A further development of the idea of Ref. 2 allowing for the $V-T$ relaxation[1,3–6] has led to the establishment of an analytic theory describing the steady-state distribution of molecules between the vibrational levels.

We shall give an analytic theory of the transient processes of the establishment and relaxation of the vibrational distribution function under conditions far from equilibrium.

The evolution of the vibrational distribution function $f(v)$ can be described by a system of kinetic equations

$$\partial f/\partial t=\Pi_{v+1}-\Pi_v+i_v, \qquad (1)$$

where Π_{v+1} is the flux of vibrational populations in the space of vibrational numbers in a section between the v-th and $(v+1)$-th levels; i_v is the excitation frequency of the v-th level by external sources. The flux Π_{v+1} can be expressed in terms of the frequencies of the $V-V$ exchange $Q_{v+1,v}^{v',v'+1}$ and the frequencies of the collisional and radiative relaxations P_v and A_v:

$$\Pi_{v+1}=\sum_{v'}(Q_{v+1,v}^{v',v'+1}f_{v+1}f_{v'}-Q_{v,v+1}^{v'+1,v'}f_vf_{v'+1})+(P_{v+1}+A_{v+1})f_{v+1}. \qquad (2)$$

Application of a familiar theory[3,5,6] makes it possible to simplify considerably the expression for the flux in the case of a state far from equilibrium. The main assumption of this theory,[3,5,6] which is the smallness of the change in f_v in the $|\Delta v|\lesssim\Delta v_Q$ case [Δv_Q is the $V-V$ exchange radius representing a reduction in the probability of exchange in processes with an energy defect (as a rule, we have $\Delta v_Q\approx 1-3$)], makes it possible to adopt a continuous variable v, use an analog of the Fokker–Planck approximation, and obtain the following differential form for Π_{v+1}:

$$\Pi(v)=\nu\left\{\frac{\partial}{\partial v}\left[(v+1)^2f^2(v)\left(1-\frac{T}{2\Delta E}\frac{d^2\ln f}{dv^2}\right)\right]\right.$$
$$\left.+2\mu\left(\exp\{\delta_{V-T}v\}+\frac{A_{10}}{P_{10}}\right)f(v)(v+1)\right\}. \qquad (3)$$

Specifically, we can use the following approximation for the $V-V$ exchange rate:[1,5,6]

$$Q_{v+1,v}^{v',v'+1}=Q_{10}(v+1)(v'+1)\exp(-\delta_{V-V}|v-v'|), \qquad (4)$$

where δ_{V-V} is the reciprocal $V-V$ exchange radius[1,5,6] depending on the type of molecule and gas temperature

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