

ROTATIONAL RELAXATION TIME AND TRANSFER
COEFFICIENTS IN A DIATOMIC GAS

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Two independent definitions of relaxation time are widely used today. In the first case the general expression for the temperature dependence of the relaxation time, $\tau_{R1}(T)$, is obtained by using the Chapman—Enskog iteration method to solve the Boltzmann equation for a gas of particles which possess internal degrees of freedom [1]. In the second case the relaxation time, $\tau_{R2}(T)$, is found directly from the relaxation equation by calculating the rate of increase of the internal energy of the molecules which originally were not internally excited [2].

In the classical description of the rotational relaxation of a gas of homonuclear diatomic molecules it is necessary to specify some model of the intermolecular interaction which can be used for calculating the redistribution of the rotational and translational energies upon collision. The main disadvantage of the rough-sphere, loaded-sphere, spherocylinder, and ellipsoid models is that the real intermolecular interaction potential is replaced with the potential of rigid frames of different shape. As a result, the average number of collisions calculated by means of these models which is required to put the system into equilibrium with respect to the rotational degrees of freedom, $Z_{R1}(T) = \tau_{R1}/\tau$, where τ is the translational relaxation time, is independent of the temperature; this contradicts the experimental data [3].

Within the framework of the Parker model [4], the interaction potential of the molecules is represented as the sum of the exponential attraction between the centers of mass and the exponential repulsion between the centers of force, placed on the internuclear axis at a distance $d^* < d$ from each other, where d is the internuclear distance. Expansion of the short-acting part of the potential in a Fourier series led to the generally accepted form of an expansion in powers of the cosines of the angles between the interatomic and intermolecular axes. The retention of only the first two terms of this expansion was justified by the fact that the anisotropy parameter $\epsilon = 2I_2(y)/I_0(y)$ is small; here $y = \alpha d^*/2$, α is the inverse radius of action of the intermolecular forces, I_0 and I_2 are modified Bessel functions. The quantity $Z_{R2}(T) = \tau_{R2}/\tau$, calculated in [4] and obtained more precisely in [5], corresponding to the plane collision of the initially unperturbed rotators, increased monotonically with the increase in temperature because of the potential well. The effect of the potential well on $Z_{R2}(T)$ in the range of temperatures tens of times as high as its depth is explained in [6] by the approximate nature of the estimates of the integrals in [4].

The problem of the redistribution of the translational and rotational energy is solved in [6] for the Parker model potential, taking account of the initial rotational excitation of the molecules colliding in the plane. In [6] the effect of the remote-acting part of the potential is manifested only in the additional acceleration of the participating entities in the region of interaction, and the calculated dependence on temperature is extremely weak.

A comparison of two-dimensional and three-dimensional calculations was carried out in [7, 8] by numerical integration of the equations of motion with the Parker potential. It was shown that in the three-dimensional case $Z_{R1}(T)$, depending on the potential parameters, is 1.5 to 3 times as high as in the plane case, and the ratio of relaxation times is independent of the temperature [7]. Thus, the transition from the two-dimensional to the three-dimensional case may be made either by introducing an additional steric factor or by an appropriate choice of the curve-fitting parameter d^* of the theory.

The potential of the pairwise exponential repulsion of individual atoms in the molecules was used in [9] as the intermolecular potential. Unlike the case of the Parker potential [4], in the expansion of the potential [9] in a series in powers of the cosines of the

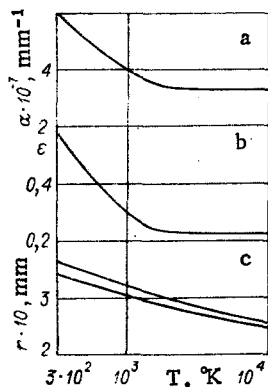


Fig. 1

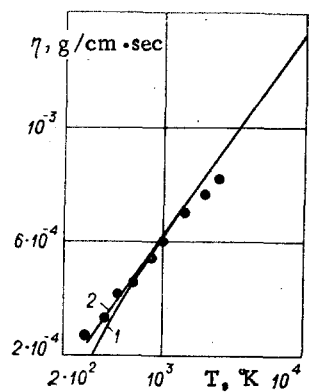


Fig. 2

angles between the interatomic and intermolecular axes, because of the large anisotropy parameter, it is no longer possible to confine the expansion to the first two terms. The numerical calculation carried out in [9] revealed that even though the remote-acting part of the potential was disregarded, $Z_{R_1}(T)$ increased monotonically with temperature. The discrepancy between the results of [4] and [9] is attributed in [9] to the assumptions adopted in [4] in solving the system of equations of motion. However, these discrepancies may be caused by the difference between the interaction potentials.

The adiabatic character of the energy exchange between the highly excited rotational states of the molecules was taken into account in [5], in which the time of rotational relaxation was determined by solving the diffusion equation for the case of ultrasound passing through the gas. The Parker model potential was used in calculating the diffusion coefficient. It was found that the time of rotational relaxation depends on the frequency of the ultrasound, taking on values about twice as large as $\tau_{R_2}(T)$.

The classical expressions for the coefficient of shear viscosity and the thermal conductivity of a gas of particles possessing internal degrees of freedom were obtained in [10] by solving the classical variant of the Boltzmann equation using the Chapman-Enskog method. The formulas presented in [10] have the form of values obtained by averaging over the parameters of the colliding pair of molecules for functions of the energy $\Delta E'$ transmitted from the translational to the rotational degrees of freedom when collision takes place and of the scattering angle χ .

The calculation of $\Delta E'$ and χ for the case of collision between rigid rotators may be carried out by using the rough-sphere, loaded-sphere, spherocylinder, and ellipsoid models. However, a comparison of the shear-viscosity and thermal-conductivity values calculated on this basis with the experimental values does not yield particularly good results [1].

In [8] $\Delta E'$ and χ were obtained by numerical integration of the two-dimensional and three-dimensional classical equations of motion with the Parker model potential. The shear-viscosity coefficients and the thermal conductivities are represented in the form of tenfold integrals and calculated by the Monte Carlo method. Because this kind of calculation is very cumbersome, the results shown correspond to only three temperature values: $T=300, 600,$ and 900°K . The calculated results agree satisfactorily with the experimental ones.

Mason and Monchick [11], who considered as the excitation the ratio of $\Delta E'$ to kT , where k is the Boltzmann constant, simplified the relations of [10]. The approximate relations given in [11] include $\tau_{R_1}(T)$ and the self-diffusion coefficient as the parameters; these can be obtained without solving the dynamic problem of the collision of particles possessing internal degrees of freedom. The relations of [11] are still being used today for calculating the transfer coefficients.

In the present study the calculation of $Z_{R_1}(T)$ and $Z_{R_2}(T)$, as well as of the coefficient of shear viscosity and the thermal conductivity, is carried out in the temperature range from 300 to $10,000^\circ\text{K}$ for nitrogen. The short-acting part of the Parker potential is used as the potential of interaction of the molecules. The distortion of the selected potential by remote-acting forces is taken into account by introducing a temperature-dependent inverse radius of action. It is proposed to use instead of $Z_{R_2}(T)$ the two-parameter quantity $Z_{R_2}(T, T_R)$, which depends not only on the temperature but also on a parameter T_R characterizing the

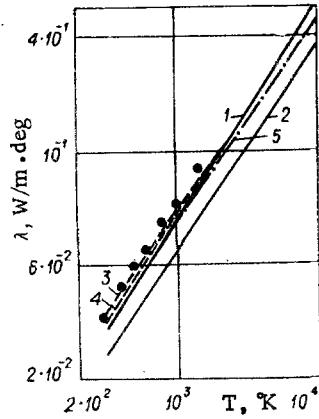


Fig. 3

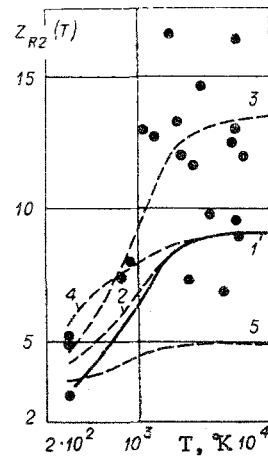


Fig. 4

initial distribution over the rotational levels. The possibility of introducing the two-parameter dependence of $Z_{R2}(T, T_R)$ is confirmed by means of an exact calculation carried out for parahydrogen in the isothermal case. The shear-viscosity and thermal-conductivity values calculated by the Chapman-Enskog method are compared with the values obtained by using the approximate relations of [11]. We carry out an analysis of the sensitivity of the calculated values to the parameters of the interaction potential.

1. We consider the problem of the redistribution of the translational and rotational energy when there is a collision between identical homonuclear molecules in a fixed plane which is at the same time the plane of rotation of each molecule. Following Parker [4], we represent the interaction potential in the form:

$$V = C \exp(-\alpha r)(1 + \varepsilon \cos 2\theta_1 + \varepsilon \cos 2\theta_2), \quad (1.1)$$

where C is a constant, r is the intermolecular distance, and θ_1 and θ_2 are the angles between the intermolecular and interatomic axes of the molecules.

The system of classical equations of motion with potential (1.1) given in [4] was solved within the framework of the theory of perturbations with respect to ε . In the zeroth approximation the rotational state of the molecules does not change as a result of the collision. In a narrow range of action of the intermolecular potential, $1/\alpha$, the centrifugal energy $mv^2b^2/2r^2$, which varies only slightly with r , in accordance with the effective-wave-number approximation [12], is replaced with the constant value $mv^2b^2/2r_0^2$, where m is the mass of an atom of the molecule, b is a target parameter, v is the velocity of relative motion of the participating entities which do not act on each other, r_0 is a parameter which takes on a value in a narrow range $1/\alpha$ around the point of rotation.

The approximations adopted enable us, in the first order of the theory of perturbations with respect to ε , to obtain analytic expressions for the resulting angular velocities of the molecules:

$$\varphi_i = -16\pi l_i \sin 2\psi_i / (\alpha^2 d^2 \text{sh}^2 \kappa_i) \quad (i = 1, 2), \quad (1.2)$$

where $l_i = \sqrt{2}p_i/d - qg/r_0$; $\psi_i = \varphi_i - \arcsin q$; $\kappa_i = 2\pi l_i / (\alpha g \sqrt{1 - q^2 + 2D/g^2 kT})$; $q = b/r_0$; $g = (\sqrt{m}/kT)v$; p_i and φ_i are the initial reduced angular momenta and initial phases counted from the direction of the initial velocity of relative motion of the molecules. The additional acceleration in the region of interaction as a result of the remote-acting forces is taken into account in (1.2) according to [12] by replacing $mv^2/2$ with $mv^2/2 + D$, where $D = 96.6^\circ\text{K}$ is the depth of the potential well [13].

The expressions for the energy $\Delta E = (2/mv^2)\Delta E'$, $\Delta E = \Delta E_1 + \Delta E_2$ and the momentum $\Delta M = \Delta M' / mvr_0$, $\Delta M = \Delta M_1 + \Delta M_2$ transferred at the time of collision from the translational to the rotational degrees of freedom take the form

$$\begin{aligned} \Delta E_i &= 128\pi^2 \varepsilon^2 l_i^2 \sin^2 2\psi_i / (\alpha^4 g^2 d^2 \text{sh}^2 \kappa_i) \\ &\quad - 16\sqrt{2}\pi \varepsilon p_i l_i \sin 2\psi_i / (\alpha^2 g^2 d \text{sh} \kappa_i), \\ \Delta M_i &= -8\pi \varepsilon l_i \sin 2\psi_i / (\alpha^2 g r_0 \text{sh} \kappa_i) \quad (i = 1, 2). \end{aligned} \quad (1.3)$$

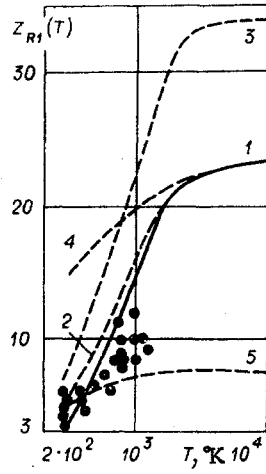


Fig. 5

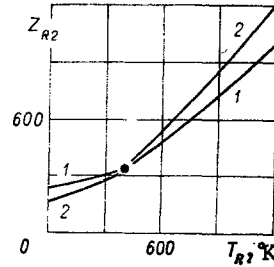


Fig. 6

The forces of attraction lead to a substantial difference in the isotropic part of the model potential of (1.1) from the real isotropic potential of interaction of the nitrogen molecules, $V_0(r)$, taken from [13], in the range $r > 3.1096 \cdot 10^{-7}$ mm. Approximating the short-acting branch of $V_0(r)$ by the exponential function $C \exp(-\alpha r)$ at each point of rotation r_p , we find the value of the parameter $\alpha(r_p) = -d \ln V_0(r) / dr |_{r_p}$. In the case when the function giving the distribution of the molecules according to energy of relative motion differs only slightly from the Maxwellian function, each r_p , and consequently each $\alpha(r_p)$, can be referred to the maximum of this function, localized around kT .

The graphs of $\alpha(T)$ and $\varepsilon(T)$ corresponding to $d^* = 0.62$ are shown in Fig. 1a and Fig. 1b, respectively.

We equate the parameter r_0 taking on a value in a narrow range $1/\alpha$ to the integral $\sqrt{\Omega^{(2,2)}}$, calculated in [13] for the exact potential $V_0(r)$. Such a choice of r_0 ensures that the transfer coefficients calculated in [13] are equal to the transfer coefficients of a gas of solid spheres of radius $r_0/2$. The graphs of $r_0(T)$ and $r_p(T)$ are shown in Fig. 1c.

As is known, the angle of elastic scattering for a short-acting potential can be satisfactorily approximated by the angle of scattering of solid spheres [12]. In view of the fact that the calculated values of $\Delta E'$ are much smaller than kT , the calculation of the angle of scattering is carried out on the assumption that the transfer of energy from the translational to the rotational degrees of freedom takes place instantaneously at the point r_0 . As a result, we have

$$\chi = \beta - \gamma, \quad \gamma = \arcsin \left(\frac{\sin \beta - \Delta M}{\sqrt{1 - \Delta E}} \right), \quad (1.4)$$

where $\beta = \arcsin q$ is the angle between the vector \mathbf{v} and the vector drawn from the center of scattering to the point r_0 .

In the τ -approximation the process of establishing equilibrium with respect to the rotational degrees of freedom is described by the relaxation equation establishing the exponential approximation to equilibrium with respect to time [2]:

$$d\varepsilon_R/dt = (\varepsilon_R^0 - \varepsilon_R) / \tau_R, \quad (1.5)$$

where ε_R is the rotational energy per molecule and ε_R^0 is its equilibrium value. In general, (1.5) holds for small deviations from equilibrium $(\varepsilon_R^0 - \varepsilon_R) / \varepsilon_R^0 \ll 1$; $\tau_{R2}(T)$ is determined from (1.5) as the ratio of ε_R^0 to the rate of growth of the energy of the initially unexcited rotators [2]. In the case considered here, this rate can be determined by averaging (1.3), in which we must first set $p_1 = p_2 = 0$:

$$Z_{R2}(T) = \frac{4}{\pi \eta_0} p \tau_{R2}(T), \quad p \tau_{R2}(T) = \frac{5}{I} \left(\frac{\alpha^2 d r_0}{128 \pi \varepsilon} \right)^2, \quad (1.6)$$

where p is the gas pressure; $I = \frac{2}{(2\pi m k T)^{1/2}} \int_0^{\infty} \int_0^{\infty} q^2 \frac{g^5}{8} \exp\left(-\frac{g^2}{2}\right) / \text{sh}^2 \alpha_0 b d b d g$; $\eta_0 = 5(2\pi m k T)^{1/2} / 16\pi r_0^2$;
 $\alpha_0 = \alpha_1 |_{p_1=0}$.

Let us estimate the effect of the initial distribution with respect to the rotational states, which are disregarded when we calculate $Z_{R_2}(T)$ (1.6). We assume that at time $t=0$ this distribution corresponds to the Boltzmann distribution with some temperature $T_R \neq 0$. In that case the time of rotational relaxation becomes a function not only of T but of T_R as well:

$$Z_{R_2}(T, T_R) = \frac{4}{\pi\eta_0} p\tau_{R_2}(T, T_R), \quad p\tau_{R_2}(T, T_R) = \frac{5\pi}{6^4} \frac{(1 - T_R/T)}{\tilde{T}},$$

$$\tilde{T} = \frac{2}{\pi^2} \frac{1}{(2\pi mkT)^{1/2}} \int_0^{\infty} \int_0^{\infty} \int_0^{\pi} \int_{-\infty}^{+\infty} \Delta \tilde{E} \exp\left(-\frac{g^2 + p_1^2 + p_2^2}{2}\right) b db \frac{g^5}{8} dg d\varphi_1 d\varphi_2 dp_1 dp_2, \quad (1.7)$$

where we must use as $\Delta \tilde{E}$ the expression (1.3), in which p_i should be replaced by $(\sqrt{T_R}/T)p_i$.

In the case of unobstructed exchange between the translational and rotational degrees of freedom $\tau \ll \tau_{R_1}(T) \ll \theta$, where θ is the characteristic time of flow, and ϵ_R^0 and ϵ_R differ from each other by a small quantity proportional to the Knudsen number. The general expression for $Z_{R_1}(T)$ is found by solving the Boltzmann equation, using the Chapman—Enskog [1]:

$$Z_{R_1}(T) = \frac{4}{\pi\eta_0} p\tau_{R_1}(T),$$

$$1/p\tau_{R_1}(T) = \frac{5}{3} \frac{2}{\pi^2 (2\pi mkT)^{1/2}} \int_0^{\infty} \int_0^{\infty} \int_0^{\pi} \int_{-\infty}^{+\infty} \Delta E^2 \exp\left[-\frac{g^2 + p_1^2 + p_2^2}{2}\right] b db \frac{g^7}{16} dg d\varphi_1 d\varphi_2 dp_1 dp_2. \quad (1.8)$$

In deriving (1.8) we determined the temperature on the basis of the total molecular energy. Formula (1.8) differs by a factor of 5/3 from the corresponding quantity obtained in determining the temperature on the basis of the kinetic energy of the molecules [2].

The general expressions for the transfer coefficients corresponding to the case of unobstructed exchange between the translational and rotational degrees of freedom are given in [8, 10]. In the case under consideration these expressions take on the form

$$\eta^{-1} = \frac{8}{5} \int \left(\sin^2 \chi - \frac{\Delta E^2}{2} \sin^2 \chi + \frac{\Delta E^2}{3} \right) \frac{g^2}{2} dw, \quad \eta_0^{-1} = \frac{16\pi r_0^2}{5 (2\pi mkT)^{1/2}},$$

$$\lambda \left(1 - \frac{Y^2}{XZ} \right) = \frac{75}{16} \frac{k}{m} \frac{1}{X} + \frac{15}{4} \frac{k}{m} \frac{Y}{XZ} + \frac{3}{4} \frac{k}{m} \frac{1}{Z},$$

$$X = \frac{5}{2} \frac{1}{\eta} + \frac{5}{4} \frac{1}{p\tau_{R_1}(T)}, \quad Y = \frac{3}{4} \frac{1}{p\tau_{R_1}(T)},$$

$$Z = \frac{3}{2} \frac{1}{\rho D_0} + \int \left\{ \frac{3}{4} g^2 \Delta E^2 + (p_1^2 - p_2^2) [p_1^2 \cos \chi_0 - (p_1^2 + g^2 \Delta E_1) \sqrt{1 - \Delta E \cos \chi}] \right\} dw,$$

$$\frac{1}{\rho D_0} = \frac{8}{3} \int (1 - \cos \chi_0) dw, \quad \lambda_0 = \frac{15}{8} \frac{k}{m} \eta_0,$$

$$\int () dw = \frac{1}{\pi^2 (2\pi mkT)^{1/2}} \int_0^{\infty} \int_0^{\infty} \int_0^{\pi} \int_{-\infty}^{+\infty} () \exp\left[-\frac{g^2 + p_1^2 + p_2^2}{2}\right] \frac{g^5}{8} dg b db d\varphi_1 d\varphi_2 dp_1 dp_2. \quad (1.9)$$

In (1.9) η and η_0 are the coefficients of shear viscosity corresponding to rotationally inelastic and elastic collisions; λ and λ_0 are the corresponding values of the thermal conductivity; ρ is the density of the gas; D_0 is the self-diffusion coefficient of the elastically colliding molecules. In the expression for Z we can distinguish explicitly the term $(3/2)\rho D_0$, corresponding to the three-dimensional diffusive transfer of rotational energy, $\cos \chi_0 = -\cos \beta_0$.

The simplest approximation, generally used in calculating the transfer coefficients, is

$$\lambda = \left(\frac{3}{4} \frac{k}{m} f_{tr} + \frac{1}{2} \frac{k}{m} f_{in} \right) \eta, \quad (1.10)$$

where $\eta = \eta_0$ [1]. Aiken, using elementary ideas about the mean free path and taking account of the correlation between the kinetic energy of a molecule and its velocity, obtained the following values for the coefficients: $f_{tr}^e = 5/2$, $f_{in}^e = 1$ [1].

Mason and Monchick [11], analyzing the relations (1.9), set $\Delta E = 0$ in the first approximation. The resulting expression for the thermal conductivity coincided with (1.10), in

which, however, $f_{tr}^1 = 5/2$, $f_{in}^1 = \rho D_0 / \eta$, where $\eta = \eta_0$. The first approximation in the method of [11] takes account of the diffusive transfer, but it disregards the relaxation of the rotational energy. The relaxation was taken into account partially in the next, second, approximation, in which the term for Z contains not only $(3/2)\rho D_0$ but also the first term of the sum under the integral sign. As a result, the expressions for the coefficients f_{tr}^2 and f_{in}^2 from (1.10) have the form

$$f_{tr}^2 = \frac{5}{2} \left[1 - \frac{1}{2} \left(1 - \frac{2}{5} \frac{\rho D_0}{\eta} \right) \frac{\eta}{p \tau_{R1}} \right], \quad f_{in}^2 = \frac{\rho D_0}{\eta} \left[1 + \frac{3}{4} \left(1 - \frac{2}{5} \frac{\rho D_0}{\eta} \right) \frac{\eta}{p \tau_{R1}} \right].$$

In the second approximation $\sin^2 \chi$ was approximated by its value averaged over the unit sphere, which was equal to $2/3$; thus, $\eta = \eta_0$.

2. Figure 1 shows the graphs of $\alpha(T)$, $\varepsilon(T)$, or $r_0(T)$ corresponding to $d^* = 0.62$, which were used for calculating the rotational relaxation times and the transfer coefficients. Sixfold integrals were calculated at 200 points of the range of temperatures under investigation, using the Monte Carlo method, with 4000 tests at each point. A smooth curve showing variation with temperature was drawn through the points by means of piecewise cubic interpolation splines of defect 1 with smoothing [14]. The resulting estimated accuracy of the calculations is 1.5%. At the lower boundary of the temperature range the accuracy of the calculation is somewhat lower, since the higher orders of the theory of perturbations with respect to ε make a substantial contribution.

Curves 1 and 2 in Fig. 2 show η and η_0 , respectively, as given by (1.9), while the dots indicate the experimental points of [15]. The discrepancy between η and η_0 reaches values as high as several percent in the low-temperature region; for temperature $T > 1000^\circ K$ they no longer exceed the experimental error. Curves 1 and 2 in Fig. 3 show λ and λ_0 , respectively, as given by (1.9). The dashed curves 3 and 4 correspond to Mason and Monchick's first and second approximations, λ_1 (formula (1.10) with f_{tr}^1 and f_{in}^1) and λ_2 , respectively. The dot-and-dash curve 5 was calculated in the Aiken approximation λ_e , while the dots indicate the experimental results of [15]. The discrepancy between λ and λ_1 , which differs from λ_0 because the diffusive transfer of rotational energy has been taken into consideration, amounts to several percent in the low-temperature range. Taking account of the relaxation of the rotational energy in λ_2 improves the agreement with the exact calculation. In the high-temperature range, $T > 1000^\circ K$, the amount by which λ differs from λ_1 and λ_2 does not exceed the experimental error; λ is greater than λ_e in the entire range of temperatures investigated.

Numerical calculations showed that the deviation of η from η_0 and that of λ from λ_2 and λ_1 in the low-temperature region is due solely to the difference between the scattering angle for rotationally inelastic collision and the elastic-scattering angle χ_0 . The parameters D , α , and d^* of the potential influence the value of this deviation in different degrees. The variation of D , which is responsible for the additional acceleration of the participating entities in the region of interaction, does not lead to any change in η , λ , and λ_2 that exceeds the accuracy limits of the calculation. If the parameters α and d^* are increased, there is a decrease of several percent in η , λ , and λ_2 .

The approximation selected in this study for the isotropic part of the potential of interaction of the molecules predetermined the nature of the variation of η_0 and λ_0 , and hence η and λ , as functions of temperature. Thus, the small discrepancy between the theoretical temperature-dependent variation of η and λ and the experimental results (see Figs. 2, 3) can be eliminated chiefly by a proper choice of the potential.

The calculation showed that over the entire temperature range investigated, $Z_{R1}(T)$ is 2 to 2.5 times as large as $Z_{R2}(T)$, irrespective of the potential parameters D , α , and d^* . This difference is apparently due to the adiabatic nature of the energy exchange between the highly excited rotational states of the molecules. The quantity $Z_{R1}(T)$ should be used for interpreting the experimental data on the scattering and absorption of ultrasound, where the effect of the ultrasound frequency on $Z_{R1}(T)$ is disregarded [5]. The quantity $Z_{R2}(T)$ should be used for interpreting the data of experiments in shock tubes. In this comparison we disregard the effect of the initial distribution according to rotational levels.

It should be noted that the available experimental data, both on ultrasound and on shock waves, differ from one another by 200-300%, which is approximately equal to the difference between $Z_{R1}(T)$ and $Z_{R2}(T)$. The experimental dispersion makes it much more difficult to choose the curve-fitting parameter of the theory, d^* . The value $d^* = 0.62$, in our opinion,

most satisfactorily interprets the totality of the experimental data both in shock tubes (Fig. 4) and in ultrasound tubes (Fig. 5); $d^* = 0.62$ is an intermediate value between the generally used values $d^* = 0.557$ [4] and $d^* = 0.66$ [6].

Curves 1 in Figs. 4 and 5 are the results of calculations performed according to formulas (1.6) and (1.8), respectively. The dots represent the experimental results found by the various authors in [5, 8]. The dashed curves 2 are the result of calculations performed according to formulas (1.6) and (1.8) for $D = 0$. Thus, taking account of the additional acceleration caused by the remote-acting forces slightly decreases $Z_{R1}(T)$ and $Z_{R2}(T)$ in the low-temperature region. The parameters α and d^* have the greatest effect on $Z_{R1}(T)$ and $Z_{R2}(T)$: a decrease in α and in d^* causes an increase in $Z_{R1}(T)$ and $Z_{R2}(T)$. The dashed curves 3 correspond to $d^* = 0.557$, while curves 4 and 5 correspond to the constant values $\alpha = 3.35 \cdot 10^7$ and $5.32 \cdot 10^7 \text{ mm}^{-1}$, respectively. It should be noted that for constant α both $Z_{R1}(T)$ and $Z_{R2}(T)$ will remain approximately constant everywhere except at low temperatures, where taking account of the additional acceleration of the participating entities caused by the remote-acting forces reduces them only slightly. Thus, within the framework of the model described above, the experimentally observed increase in $Z_{R1}(T)$ and $Z_{R2}(T)$ with increasing temperature is due practically completely to the distortion of the exponential repulsion caused by remote-acting forces, which is taken into account by using the temperature-dependent variation of the parameter α .

The quantity $Z_{R2}(T, T_R)$, calculated by (1.7) for $T = 1000^\circ\text{K}$, decreases from 6.5 for $T_R = 0$ to 1.6 for $T_R = 800^\circ\text{K}$.

3. For an answer to the question of which of the relaxation times $\tau_{R2}(T)$ and $\tau_{R2}(T, T_R)$ can be used to give a more accurate description of the manner in which the system approaches equilibrium, we must compare the solution of Eq. (1.5) with the exact solution obtained by integrating the kinetic equations for the occupancies of the rotational states.

The system of kinetic equations for the occupancies n_j of the individual rotational levels j was solved in our study for parahydrogen at a constant temperature $T = 400^\circ\text{K}$. In the calculation, we used the constants of the rates of rotational transfers calculated in [16] within the framework of the effective-potential method, with $r_0^2 = 8.55 \cdot 10^{-14} \text{ mm}^2$ from [3]. The quantities $\tau_{R2}(T)$ and $\tau_{R2}(T, T_R)$ obtained on the basis of (1.5) were compared with the exact value $\tau_{R2}^{\text{exact}}(T, T_R)$, determined by the relation

$$\varepsilon_R(\tau_{R2}^{\text{exact}}) = \varepsilon_R^0(1 - e^{-1}) + \varepsilon_R(0)e^{-1}, \quad (3.1)$$

where $\varepsilon_R^0 = \sum B_j(j+1)n_j^0$; $\varepsilon_R(0) = \sum B_j(j+1)n_j(0)$; n_j^0 and $n_j(0)$ are the Boltzmann occupancies of the j -th level with temperatures T and T_R , respectively; B is the rotational constant.

The results of the calculation are shown in Fig. 6; $Z_{R2}(T, T_R)$ for $T = 400^\circ\text{K}$ is given by curve 1, and the result of the exact calculation using (3.1) is given by curve 2. The point $T_R = 0$ of curve 1 corresponds to $Z_{R2}(T)$. As in the case of the rotational relaxation of nitrogen, investigated above, we find a fairly strong dependence of the relaxation time on T_R , and the use of a two-parameter quantity markedly improves the approximate calculation obtained with (1.5). The results shown indicate that the initial distribution according to rotational levels must be taken into account within the framework of the τ -approximation.

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LITERATURE CITED

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DYNAMICS OF IMPULSIVE METAL HEATING BY A
CURRENT AND ELECTRICAL EXPLOSION OF CONDUCTORS

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Most studies of electrical explosion are of an experimental nature and are oriented toward solution of concrete practical problems. In particular, exploding conductors are used as circuit breakers in high power inductive energy storage devices, which are important components of many thermonuclear projects. Electrical explosion is of special interest in attempts to realize variants of so-called inertial thermonuclear synthesis, in which the electrical energy stored in a capacitive storage bank is transferred by a collapsing metal shell without intermediate conversion into light or energetic particles.

Simulation of the processes occurring in impulsive heating of conductors by a current is also of interest in connection with certain experimental behavior which appears anomalous. Namely, it appears that certain phenomenological characteristics of the medium are dependent not only on the thermodynamic variables, but also on the time derivatives of the latter. Thus the specific internal energy [1] and the temperature for commencement of fusion (at constant pressure) [2] become functions of the rate of temperature change; the development of anomalies in conductivity [3] and other properties has been discussed. We are concerned here with experiments having heating times t_h greater than the minimum sound time $t_s = 2r/c_s$ (where r is the conductor radius and c_s is the speed of sound) and the characteristic magnetic diffusion time $t_m = 4\pi\sigma r^2/c^2$ (where σ is the conductivity and c is the speed of light). It is assumed that the first condition ($t_h \gg t_s$) ensures uniformity of the mass density distribution over section, while the second ($t_h \gg t_m$) ensures uniformity of current density, Joulean heat source power, and temperature. However there exist estimates and experimental data which indicate that great care must be used in applying these assumptions in cases where anomalies are present.

Moreover, there is an experimental result available which in the present authors' opinion indicates that the converse is true. This is that flexing instabilities related to axial stresses can develop in a deenergized conductor a long time after the completion of the heating stage. For example, in [4] a copper conductor 1 mm in diameter was heated for 20 μ sec, and marked instability appeared only after 100 μ sec. These facts suggest

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