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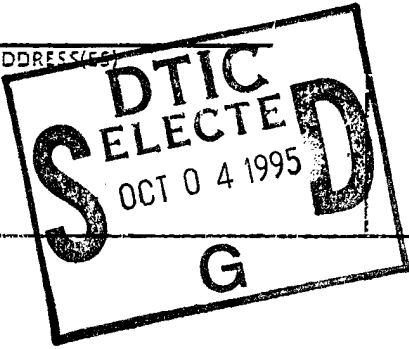
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THEORETICAL INVESTIGATIONS OF TIME-DEPENDENT BEHAVIOR OF ELECTRONS IN GASES

GRANT NUMBER:	AFOSR - F49620-92-J-0027
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1. Introduction

The major aim of our research investigations has been to develop new algorithms and the corresponding computer codes for exact numerical solutions of the time-dependent Boltzmann equation for the transport of electrons (and other charged particles) in gases subjected to external electric fields of *arbitrary* strengths. The electron velocity distribution function obtained as a solution of the Boltzmann equation is used to calculate a set of experimentally measurable swarm parameters for the transport of electrons in actual pure gases or in gas mixtures subjected to static or time-dependent external electric fields. A direct comparison of the calculated swarm parameters with the corresponding experimental values provides a useful check on the validity and accuracy of the results obtained using the present codes. It is especially useful to have a general computer program for calculating the theoretical values of the electron swarm parameters for gases for which there are, as yet, no experimental values or for which direct laboratory experiments are simply not feasible.

Using our novel algorithm we have obtained the numerical values of swarm parameters for the cases in which the external electric field is either constant or varies with time in a sinusoidal fashion, both for a pure gas as well as for a gas mixture. The external rf electric field is of the form $\mathbf{E} = E_0 \sin \omega t$ or $\mathbf{E} = E_0 \cos \omega t$, of arbitrary strength E_0 and arbitrary frequency ω . The present investigations have allowed us to analyze the relations between the frequency ω of the field and the frequency ν of collisions of the electrons with background gas particles, with number density N . These relationships can be qualitatively understood by using a simple model in which one assumes a constant collision frequency for the projectile-gas collisions. In this model the time dependence of various swarm parameters using the complete Boltzmann equation can be *analytically* solved. The whole analysis is carried out *for an arbitrary value of the ratio μ of the projectile mass to the ambient gas particle mass* so that the derived expressions are valid even for the transport of heavy ion swarms in gases subjected to external rf fields of arbitrary strength. Even though these analytical results are interesting and useful in their own right, they have been

used merely as a check on the results from the actual computer code which did not, in general, assume a constant collision frequency; in the code the energy-dependent collision frequency is determined by the actual collision cross sections used.

In the course of present work, we came across a few additional problems that needed to be investigated. For example, in order to test the versatility of our single-target-gas computer code we tried to obtain the temporal history of the behavior of charged particles other than electrons in a gas, and for this purpose we chose a positron swarm. This investigation allowed us to compare the behavior of electron swarms with that of positron swarms under similar conditions. As a part of additional investigations, we calculated the cross sections for the processes which are important for a realistic modeling of a hydrogen plasma. In this connection we have investigated the dependence of the cross sections for pure dissociation of H_2 upon the initial vibrational state of H_2 . Finally, we have also investigated the penetration probability of a quantum harmonic oscillator into the classically forbidden region in the limit of large quantum numbers using analytical methods. An expression is derived for the asymptotic form of the penetration probability, and is shown to be in good agreement with an earlier result obtained by numerical methods. The asymptotic form of the probability density in the region between the classical turning points is also presented and found to have a simple physical interpretation.

1.1 Novel method of solving the Boltzmann equation

We provide here a *very brief* summary of our algorithm for solving the Boltzmann equation exactly. The traditional Boltzmann equation used for calculating the parameters which characterize the transport of electrons injected in a neutral gas which is subjected to an external electric field E (constant or time-dependent) is

$$\frac{\partial f(\mathbf{v}, t)}{\partial t} + \mathbf{a} \cdot \nabla_{\mathbf{v}} f(\mathbf{v}, t) = R(\mathbf{v}, t) \quad , \quad (1)$$

The solution $f(\mathbf{v}, t)$ provides the (spatially homogeneous) velocity, or equivalently energy, distribution function of the electrons. Here $\mathbf{a} = -e\mathbf{E}/m$ represents the acceleration of the electrons

due to external electric field \mathbf{E} and the collision term $R(\mathbf{v}, t)$ represents the rate of change in the electron velocity distribution function due to all possible collision processes among the electrons and the ambient gas particles. The collision term $R(\mathbf{v}, t)$ itself involves integrals over the distribution function $f(\mathbf{v}, t)$ so that in its complete form, the Boltzmann equation is a time-dependent integrodifferential equation whose numerical solution, in the past, has been obtained only after making some simplifying assumptions.

In our algorithm *no expansion of any kind of the distribution function is made and no derivatives are evaluated numerically*. The proposed procedure for obtaining the time-dependent velocity distribution function is numerically stable and computationally inexpensive. In order to derive the basic equation of our algorithm we multiply Eq. (1) by a small time interval Δt and add the distribution function $f(\mathbf{v}, t)$ to it to obtain

$$f(\mathbf{v}, t) + \left(\Delta t \frac{\partial}{\partial t} + \Delta \mathbf{v} \cdot \nabla_{\mathbf{v}} \right) f(\mathbf{v}, t) = f(\mathbf{v}, t) + R(\mathbf{v}, t) \Delta t \quad , \quad (2)$$

where $\Delta \mathbf{v} = \mathbf{a} \Delta t$ is a small velocity increment. Eq. (2) can be rewritten as

$$f(\mathbf{v} + \Delta \mathbf{v}, t + \Delta t) = f(\mathbf{v}, t) + R(\mathbf{v}, t) \Delta t \quad . \quad (3)$$

Thus, the difference equation (3) is entirely equivalent to the Boltzmann equation in its physical content. We have realized [1] that the above difference equation is much simpler to solve for the time-dependent velocity distribution function than the standard integrodifferential Boltzmann equation. Furthermore, being a difference equation, Eq. (3) is more suited for numerical computations than Eq. (1). A few important advantages of our novel algorithm over the traditional techniques are:

- (i) Since our algorithm does not involve any numerical computation of partial derivatives, there is no need to invoke Courant-Levy condition for numerical stability. Thus, the time-step Δt and the velocity-step Δv can be varied almost independently.

(ii) Lack of numerical evaluation of any derivatives also makes our algorithm computationally inexpensive. Almost all of our numerical results are obtained on microcomputers or workstations.

(iii) Since no truncation of expansion of any kind of the distribution function is made in our work, the present algorithm provides swarm parameters for *any* value (that is, for both high and low values) of E/N .

1.2 The collision term

An explicit expression for the collision term $R(\mathbf{v}, t)$ has been provided by Holstein [2] in the following form:

$$R(\mathbf{v}, t) = \sum_p R_p^+(\mathbf{v}, t) - R_T^-(\mathbf{v}, t) \quad , \quad (4)$$

where

$$R_p^+(\mathbf{v}, t) = \frac{N}{v^2} \int_0^\infty v_p^2 dv_p \int_0^\pi \sin \psi d\psi \int_0^{2\pi} d\alpha v_p f(\mathbf{v}_p, t) \sigma_p(v_p, \psi) \delta(\mathbf{v} - \mathbf{g}_p(v_p, \psi)) \quad (5a)$$

represents the rate at which the projectile particles with initial speed v_p are scattered, due to the p th (p = elastic, excitation, ionization etc.) scattering process, into a velocity-space-volume element d^3v located at \mathbf{v} , and

$$R_T^-(\mathbf{v}, t) = N v f(\mathbf{v}, t) \sigma_T(v) \quad (5b)$$

represents the rate at which the projectile particles are scattered, due to all possible collision processes, out of the velocity-space-volume element d^3v located at \mathbf{v} . Naturally $\sigma_p(v_p, \psi)$ is the differential cross section for the p th collision process, and $\sigma_T(v)$ is the integrated total scattering cross section. The energy conserving delta-function relates the initial speed v_p to the final speed v for the p th collision process via the function $\mathbf{g}_p(v_p, \psi)$ which is defined by the relationship

$$\mathbf{v} = \mathbf{g}_p(v_p, \psi).$$

ψ is the scattering angle. Figure 1 shows the relationship among various angles as well as directions of relevant vector quantities. For example, the direction of \mathbf{v}_p can be specified with respect to either $\hat{\mathbf{v}}$ or $\hat{\mathbf{z}}$. These two specifications imply

$$d^3v_p = v_p^2 dv_p \sin \theta_p d\theta_p d\phi_p = v_p^2 dv_p \sin \psi d\psi d\alpha \quad (6a)$$

Also, $\cos \psi = \cos \theta \cos \theta_p + \sin \theta \sin \theta_p \cos \phi_p$ (6b)

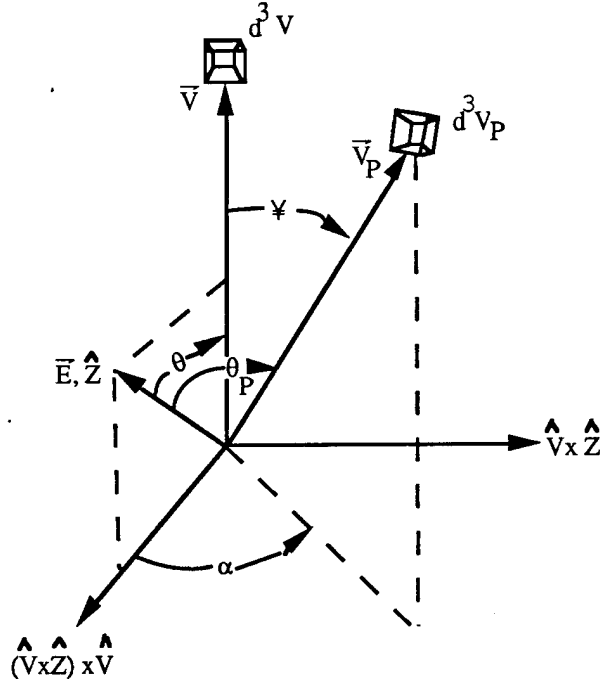


Fig. 1: Geometry used in the discussion of the collision term.

For elastic collisions ($p = e$) of projectiles of mass m incident on gas particles (of mass M) at rest, we obtain from simple kinematics (simply using conservation of energy and momentum),

$$v = v_e q(\psi) \equiv g_e(v_e, \psi) \quad (7)$$

Here $q(\psi) = \frac{(1 - \mu^2 \sin^2 \psi)^{1/2} + \mu \cos \psi}{1 + \mu}$, (8a)

and $\mu = m/M$. For small μ (for example, for electron or positron swarms in atomic and molecular gases) we can approximate

$$q(\psi) \equiv 1 - \mu (1 - \cos \psi) \quad (8b)$$

Now, no matter what simplifying assumptions one makes for obtaining a solution of Eq. (1), ultimately one will compute, for direct comparison with the corresponding experimental values, various transport or swarm parameters (such as the average energy of the projectile particles in the charged beam, the drift and diffusion rates of the beam particles in the ambient gas, the rates of excitation and ionization of the ambient gas particles by the impact of the charged beam particles etc.), which are expressed as integrals involving the distribution function $f(\mathbf{v}, t)$. A typical swarm parameter will be the expectation value of a function $g(\mathbf{v}) = g(v, \theta, \phi)$, which itself does not depend on time explicitly:

$$G(t) = \langle g(\mathbf{v}) \rangle = \frac{\int_0^{\infty} v^2 dv \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi g(v, \theta, \phi) f(v, \theta, t)}{n(t)}, \quad (9)$$

where $n(t) = 2\pi \int_0^{\infty} v^2 dv \int_0^{\pi} f(v, \theta, t) \sin \theta d\theta$ is the number density of projectiles and, in the

case of elastic collisions only, $n(t)$ is independent of time and can be normalized to 1 for convenience. Note that $f(v, \theta, t)$ is azimuthally symmetric since \mathbf{E} will be taken to be along the \hat{z} axis.

1.3 Relation between the field frequency ω and the collision frequency ν .

Because of the potential applications of a hydrocarbon-rare-gas mixture, we chose to investigate the transport of electrons in a mixture of gaseous methane and argon with the ratio of the number densities of CH_4 and Ar always maintained at 0.05. In the collision term of the Boltzmann equation we included the cross sections for elastic, vibrational excitation and ionization processes for methane, and for the elastic, excitation and ionization processes for argon. Using the numerical electron velocity distribution function we calculated, as a function of time, various swarm parameters such as the transverse diffusion coefficient, drift velocity and average energy of the electron swarm, rates of ionization and excitation of the background gas mixture by electron impact, frequencies of collisions of electrons with ambient gas targets, etc. For brevity of

presentation, we will only show the time-dependence of a single swarm parameter, namely, the average energy of electrons in the swarm. In all presentations, the initial (at $t = 0$) velocity distribution of the electrons in the swarm is assumed to be a Maxwellian distribution with an average energy of 10 eV. Also, at $t = 0$, various collision frequencies, defined as $\nu_p = \langle N\sigma_p v \rangle$ ($p = \text{elastic, excitation, ionization, etc.}$), are calculated for both methane and argon using the Maxwellian distribution function for electrons. The largest and the most relevant of these frequencies, in the present mixture, is the frequency of elastic collisions of electrons with argon. Note that the electron velocity distribution function, and consequently the collision frequencies, varies with time; however, at all times the frequency of elastic collisions of electrons with argon remains as the dominant collision frequency. In the present investigations, we have varied ω while keeping ν fixed. The results of these investigations, shown in fig. 2, provide insight in the time-dependent behavior of electron swarms in gases subjected to external rf electric fields.

Fig. 2, consisting of five frames labeled (a) to (e), shows the temporal evolution of the average electron energy in the methane-argon mixture with the value of the field frequency ω increasing from fig. 2(a) to fig. 2(e). The set of parameters belonging to this figure are: $E_0 = 744$ V/cm, the total gas density $N = 3.72 \times 10^{16} \text{ cm}^{-3}$, $E_0/N = 2$ kTd, field frequency $\omega = 1.0 \times 10^8$ Hz, $\nu_{\text{max}} = 5.80 \times 10^9 \text{ sec}^{-1}$, $N(\text{CH}_4) = 1.77 \times 10^{15} \text{ cm}^{-3}$, $N(\text{Ar}) = 3.54 \times 10^{16} \text{ cm}^{-3}$ and $N(\text{CH}_4):N(\text{Ar}) = 1:20$. On advancing from fig. 2(a) to fig. 2(e), the electric field frequency ω is increased while keeping E_0 , N and the ratio $N(\text{CH}_4):N(\text{Ar})$ fixed. In figs. 2(a) and 2(b) the collision frequency ν is larger than the field frequency ω ; in fig. 2(c) the collision frequency ν is comparable to the field frequency ω and in figs. 2(d) and 2(e) the collision frequency ν is less than the field frequency ω . Results in fig. 2 allow us to make the following conclusions:

- We observe, from figs. 2(a) and 2(b), that when collision frequency ν is larger than the field frequency ω , the average of the oscillating equilibrium values of the electron energy is more than the initial electron energy (which, in the present case, is 10 eV at $t = 0$) leading to the

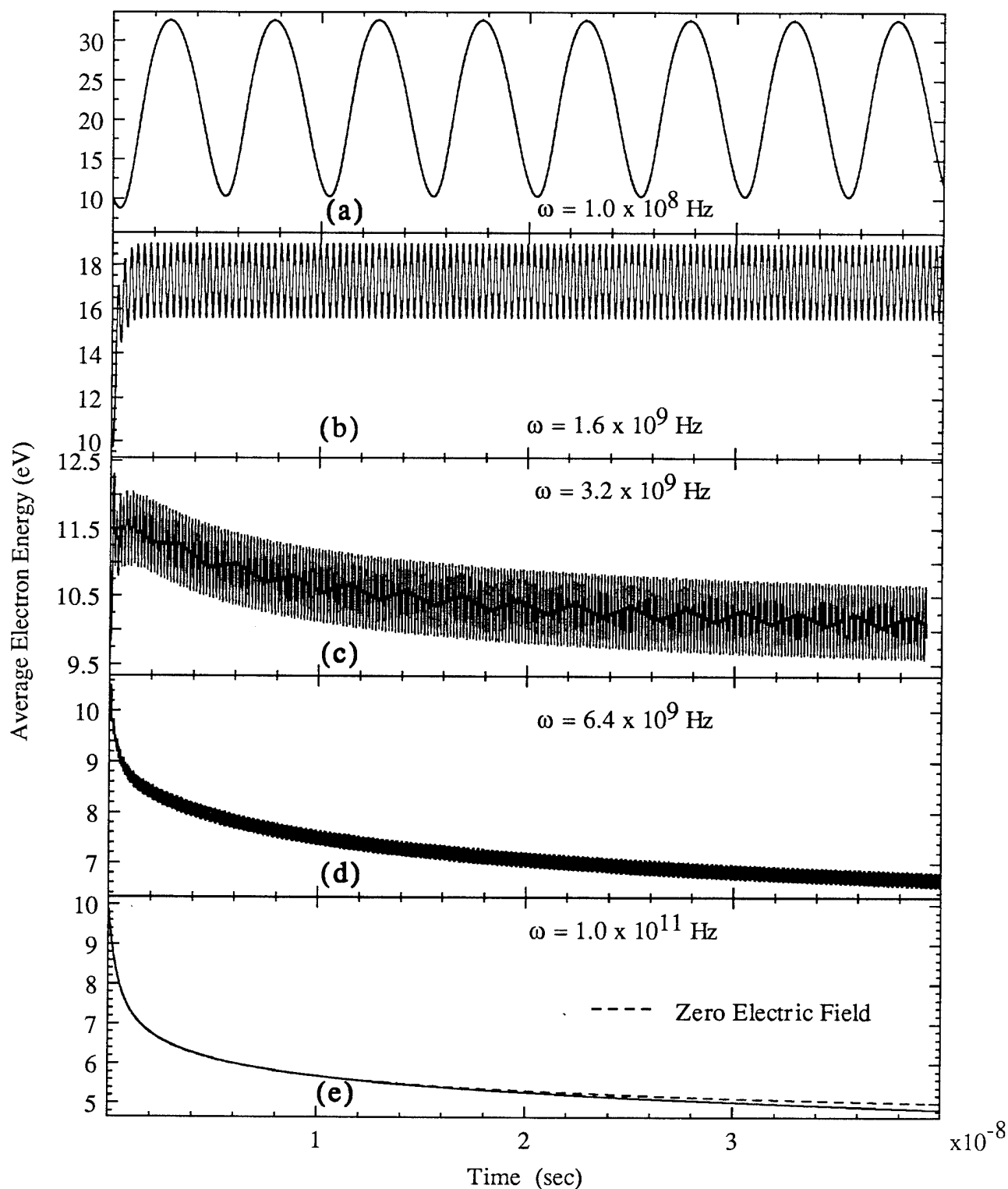


Fig. 2: Temporal evolution of the average energy of an electron swarm in a methane-argon mixture subjected to an external rf electric field for different values of the field frequency, ω .

microwave heating of the electron swarm. For ν less than ω (see figs. 2(d) and 2(e)) the electron swarm loses energy to the background gas particles.

- As the frequency ω of the field is increased, the amplitude of the oscillations in the average electron energy is reduced (compare figs. 2(a) through 2(e)). Furthermore, for very high values of ω , the average electron energy behaves (see fig. 2(e)) in the same manner as in the absence of external field. Both of these facts can be physically understood by realizing the origin of oscillations in the time-dependence of the average electron energy. Change in the average energy of the electrons is caused by collisions as well as by the external electric field; the external rf field, during its one full cycle, both accelerates as well as decelerates the electrons so that the average energy of electrons exhibits the oscillatory behavior. As the field frequency ω increases (and, therefore, the period decreases) the time available for the electrons to be accelerated or decelerated by one cycle of the field is reduced which leads to a diminished amplitude of the oscillation in the time-dependence of the average electron energy. At extremely high frequency of the field (or very small period of oscillation of the field), a typical electron makes almost no collisions during one period and, furthermore, both acceleration and deceleration of the electron by the field cause no net change in the velocity of the electron -- any change in the velocity of the electron occurs due to collisions only. Thus, in fig. 2(e) where ω is much larger than ν the average electron energy behaves as if there is no external field. A physical understanding of these results can be obtained using a simple model (see sec. 1.4)

The investigations of electron transport in a gas mixture have demonstrated that the electron swarm parameters depend sensitively on the relative values of the electron collision frequency ν and the external field frequency ω . Such investigations are important in developing a *tailor-made* mixture of gases with a pre-chosen behavior for electron transport in them.

1.4 Constant Collision Frequency Model.

While developing our computer code for the case of a sinusoidally varying time-dependent electric field, $\mathbf{E} = \hat{z} E_0 \cos(\omega t)$, we intended to consider simple cross sections in the collision

term such that the complete time-dependence of the corresponding swarm parameters, $G(t)$, can be exactly obtained analytically. These analytical expressions for the time-dependent swarm parameters will, then, provide useful checks on the correctness of the numerical results obtained from our general computer code with time-dependent electric field. With this thought in mind we started with the case where one only has isotropic elastic scattering of electrons, positrons or heavy ions by atomic and molecular targets with a constant frequency ν . Then

$$\nu = N \nu \sigma_T(\nu) = 4\pi N \nu \sigma_e(\nu, \psi) \quad , \quad (10)$$

$$R_e^+(\nu, t) = \frac{\nu}{4\pi\nu^2} \int_0^\infty v_e^2 dv_e \int_0^\pi \sin \psi d\psi \int_0^{2\pi} d\alpha f(\mathbf{v}_e, t) \delta(\nu - \nu_e q(\psi)) \quad (11a)$$

and

$$R_e^-(\nu, t) = \nu f(\nu, t) \quad . \quad (11b)$$

Now we can write the differential equation satisfied by the swarm parameter $G(t)$ [with $n(t)$ normalized to 1] simply by differentiating Eq. (9),

$$\frac{dG(t)}{dt} = \int_0^\infty \nu^2 d\nu \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi g(\nu, \theta, \phi) \frac{\partial f(\nu, \theta, t)}{\partial t} \quad . \quad (12)$$

Substituting for $\frac{\partial f}{\partial t}$ from the Boltzmann equation (1), taking $\mathbf{a} = q\mathbf{E}/m$ to be along the z-axis and using integration by parts, we obtain

$$\frac{dG(t)}{dt} = -a \left\langle \left[\frac{\partial g(\nu, \theta, \phi)}{\partial \theta} \frac{\sin \theta}{\nu} - \cos \theta \frac{\partial g(\nu, \theta, \phi)}{\partial \nu} \right] \right\rangle + \nu \left\{ \frac{dG_{1R}(t)}{dt} - \langle g(\nu, \theta, \phi) \rangle \right\} \quad , \quad (13)$$

where, as before, $\langle \dots \rangle$ represents the expectation value and

$$\nu \frac{dG_{1R}(t)}{dt} = \int_0^\infty \nu^2 d\nu \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi g(\nu, \theta, \phi) R_e^+(\nu, t) \quad . \quad (14)$$

Next, substituting $R_e^+(\nu, t)$ from Eq. (11a) into Eq. (14), using (6a) and using the delta function to carry out the ν -integration, we obtain

$$\frac{dG_{1R}(t)}{dt} = \int_0^\infty v_e^2 dv_e \int_0^\pi \sin \theta_e d\theta_e \int_0^{2\pi} d\phi_e H(\nu_e, \theta_e, \phi_e) f(\mathbf{v}_e, t) \equiv \langle H(\nu, \theta, \phi) \rangle \quad , (15)$$

where the function H is given by

$$H(v_e, \theta_e, \phi_e) = \frac{1}{4\pi} \int_0^\pi \sin \theta \, d\theta \int_0^{2\pi} d\phi \, g(v_e, \theta, \phi) \quad , \quad (16)$$

and ψ is related to θ , θ_e and ϕ_e via Eq. (6b). Thus, we obtain our principal result, namely,

the first-order ordinary differential equation satisfied by a swarm parameter $G(t)$:

$$\frac{dG(t)}{dt} \equiv \frac{d\langle g(v, \theta, \phi) \rangle}{dt} = -a \left\langle \left[\frac{\partial g(v, \theta, \phi)}{\partial \theta} \frac{\sin \theta}{v} - \cos \theta \frac{\partial g(v, \theta, \phi)}{\partial v} \right] \right\rangle + v \langle H(v, \theta, \phi) - g(v, \theta, \phi) \rangle \quad , \quad (17)$$

where $H(v, \theta, \phi)$ is given by equation (16). As we will see now, there are several important cases in which the differential equation (17) can be solved exactly. In all these cases we will take the external electric field to be sinusoidally time-dependent, that is, $\mathbf{E} = \hat{\mathbf{z}} E_0 \cos(\omega t)$, or equivalently, $a = a_0 \cos(\omega t)$. We consider two specific examples:

(a) Drift velocity of electrons.

In this case $g(v, \theta, \phi) = v \cos \theta$, and $\langle g(v, \theta, \phi) \rangle = v_d(t)$, the drift velocity. Using Eqs.

(16), (6b) and (8) together, we get, in this case,

$$H(v_e, \theta_e, \phi_e) = \frac{\mu}{3(1+\mu)} v_e \cos(\theta_e).$$

The differential equation (17), now, becomes

$$\frac{dv_d(t)}{dt} = +a_0 \cos(\omega t) - \bar{v} v_d(t) \quad , \quad (18)$$

where $\bar{v} = (1 - \lambda) v$ and $\lambda = \frac{1}{3} \left(\frac{\mu}{1 + \mu} \right)$. This differential equation can be solved exactly; the

solution is

$$v_d(t) = v_d(0) \exp\{-\bar{v} t\} - A [\bar{v} \{\exp(-\bar{v} t) - \cos(\omega t)\} - \omega \sin(\omega t)], \quad (19a)$$

$$\text{with } A = \frac{a_0}{\bar{v}^2 + \omega^2} \quad . \quad (19b)$$

As a special case, for a dc electric field ($\omega = 0$), one has

$$v_d(t) = v_d(0) \exp\{-\bar{v} t\} + \frac{a_0}{\bar{v}} [1 - \exp(-\bar{v} t)] \quad . \quad (20)$$

In the absence of collisions ($v = 0$) Eq. (20) reduces to

$$v_d(t) = v_d(0) + a_0 t \quad , \quad (21)$$

which is consistent with the simple equation of kinematics.

(b) Average energy of electrons.

For the case of average energy of electrons, $g(v, \theta, \phi) = \frac{1}{2} m v^2$ and $\langle g(v, \theta, \phi) \rangle = \epsilon(t)$.

For this case, we obtain from Eq. (16) [using (6b) and (8)],

$$H(v_e, \theta_e, \phi_e) = \frac{1}{2} m v_e^2 \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi q^2(\psi) \sin \theta d\theta = \frac{1}{2} m v_e^2 \left[\frac{3 - \mu^2}{3(1 + \mu)^2} \right]$$

and $\langle H(v, \theta, \phi) \rangle = \left[\frac{3 - \mu^2}{3(1 + \mu)^2} \right] \epsilon(t)$.

The differential equation for $\epsilon(t)$ now becomes

$$\frac{d\epsilon(t)}{dt} = + m a_o \cos(\omega t) v_d(t) + v \left\{ \frac{3 - \mu^2}{3(1 + \mu)^2} - 1 \right\} \epsilon(t) \quad , \quad (22a)$$

or

$$\frac{d\epsilon(t)}{dt} = + m a_o \cos(\omega t) v_d(t) - 6\lambda \bar{v} \epsilon(t) \quad . \quad (22b)$$

This differential equation for $\epsilon(t)$ can be solved exactly; the solution is

$$\epsilon(t) = \exp\{-6\lambda \bar{v} t\} \left[\epsilon(0) + m a_o \int_0^t dt' \cos(\omega t') \exp\{6\lambda \bar{v} t'\} v_d(t') \right] \quad . \quad (23)$$

After substituting $v_d(t)$ from Eq. (19) into Eq. (23) one can easily carry out the integrals and the resulting expression for $\epsilon(t)$ is

$$\epsilon(t) = \exp\{-6\lambda \bar{v} t\} [\epsilon(0) + m a_o J(t)] \quad , \quad (24a)$$

where

$$J(t) = \frac{v_d(0) - A\bar{v}}{(1 - 6\lambda)^2 \bar{v}^2 + \omega^2} I(t) + \frac{A}{4} \left[\frac{-3\lambda \bar{v}^2 + \omega^2}{9\lambda^2 \bar{v}^2 + \omega^2} \right] + \frac{A}{12\lambda} [\exp\{6\lambda \bar{v} t\} - 1] \\ + \frac{A}{4} \left[\frac{\exp\{6\lambda \bar{v} t\}}{9\lambda^2 \bar{v}^2 + \omega^2} \right] [\cos(2\omega t) \{3\lambda \bar{v}^2 - \omega^2\} + \sin(2\omega t) \{(1 + 3\lambda) \bar{v} \omega\}]$$

with

$$I(t) = \exp\{-(1 - 6\lambda) \bar{v} t\} [\omega \sin(\omega t) - (1 - 6\lambda) \bar{v} \cos(\omega t)] + (1 - 6\lambda) \bar{v} \quad . \quad (24b)$$

Again, for the case of a dc external field ($\omega = 0$), Eq. (24) simplifies to

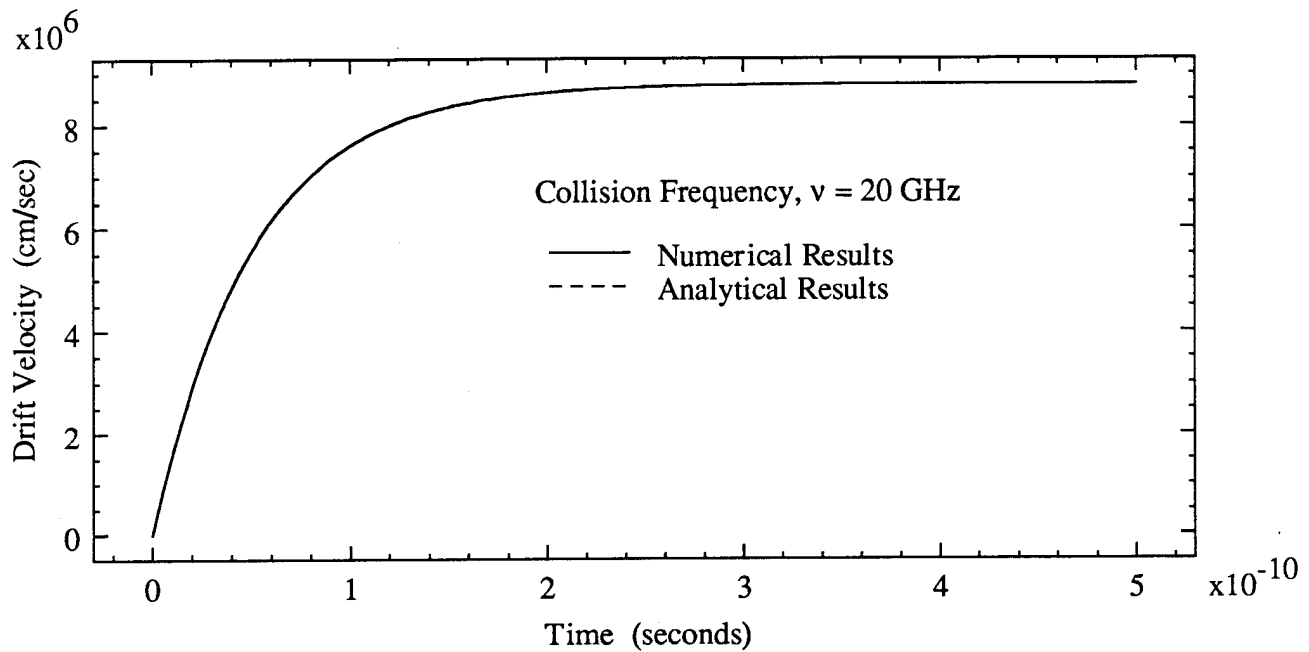


Fig. 3: Time-dependence of the electron drift velocity in a model gas, with constant collision frequency ν , subjected to an external dc electric field ($\omega = 0$).

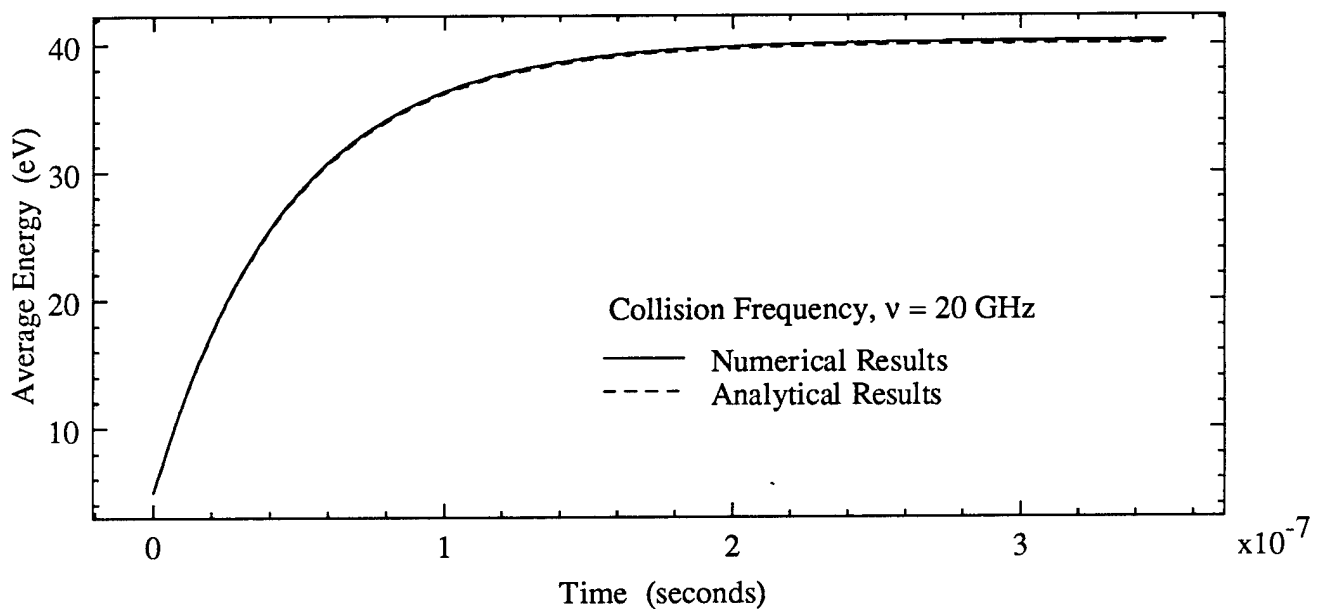


Fig. 4: Time-dependence of the electron average energy in a model gas, with constant collision frequency ν , subjected to an external dc electric field ($\omega = 0$).

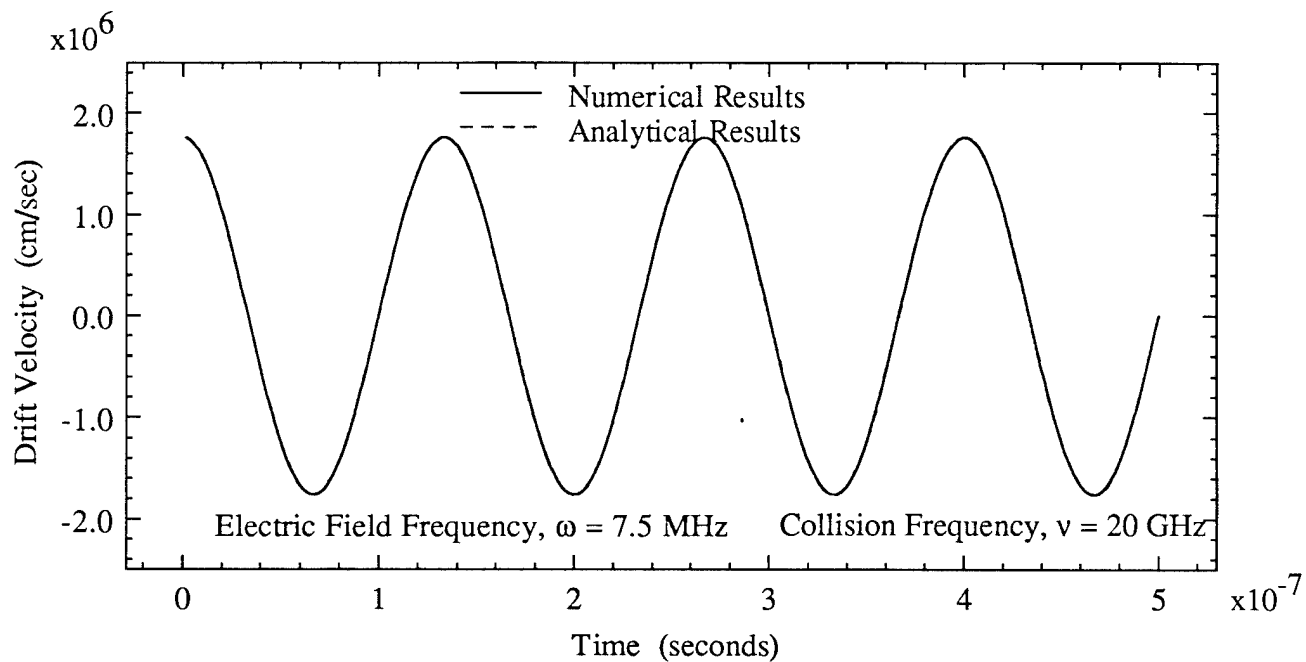


Fig. 5: Time-dependence of the electron drift velocity in a model gas, with constant collision frequency ν , subjected to an external ac electric field (frequency ω).

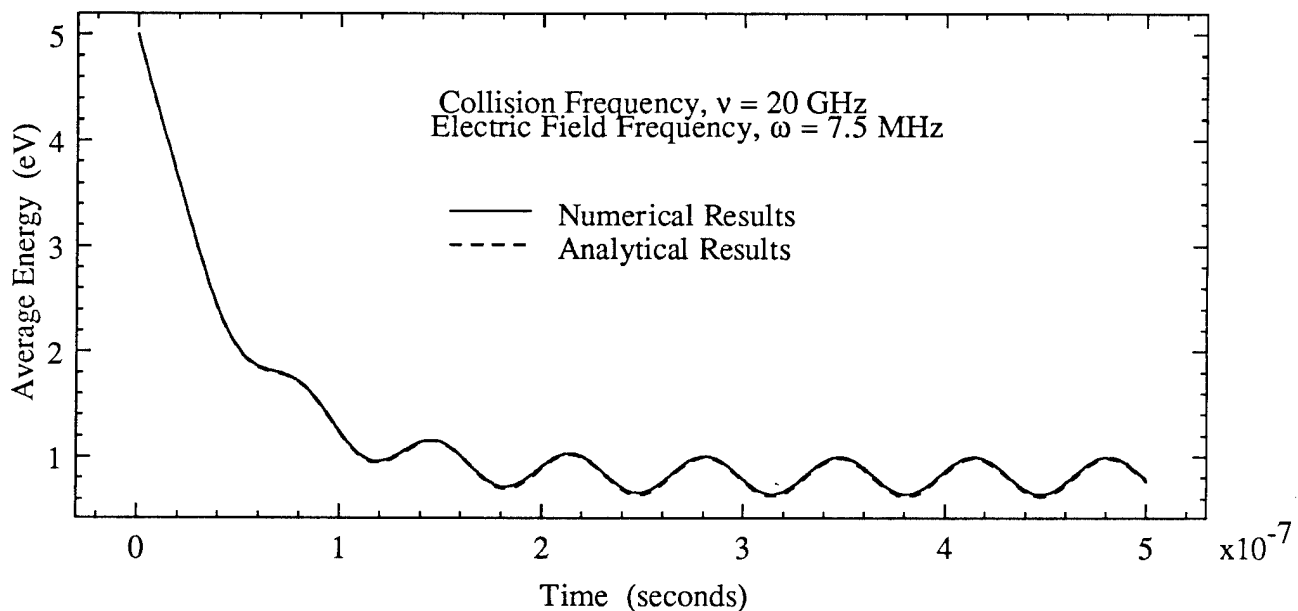


Fig. 6: Time-dependence of the electron average energy in a model gas, with constant collision frequency ν , subjected to an external ac electric field (frequency ω).

$$\begin{aligned} \varepsilon(t) = & \exp \{-6 \lambda \bar{v} t\} \varepsilon(0) + \frac{m a_o (v_d(0) \bar{v} - a_o)}{(1 - 6\lambda) \bar{v}^2} [\exp \{-6 \lambda \bar{v} t\} - \exp \{-\bar{v} t\}] \\ & + \frac{m a_o^2}{6 \lambda \bar{v}^2} [1 - \exp \{-6 \lambda \bar{v} t\}] \quad . \end{aligned} \quad (25)$$

Furthermore, in the absence of collisions ($\nu = 0$), Eq. (25) becomes

$$\varepsilon(t) = \varepsilon(0) + m a_o v_d(0) t + \frac{m a_o^2 t^2}{2} \quad , \quad (26)$$

which is consistent with Eq. (21), the simple equation of kinematics. Considerable simplification is also achieved in Eq. (24) for the case where $\mu = 0$; this is a quite reasonable assumption when electron or positron swarms are transported in atomic and molecular gases since then the ratio m/M is indeed quite small. In this case one obtains, on setting $\lambda = 0$,

$$\varepsilon(t) = \varepsilon(0) + m A [v_d(0) - A v] I(t) + m A a_o \left[\frac{1 - \cos(2\omega t)}{4} + \frac{v \sin(2\omega t)}{4 \omega} + \frac{v t}{2} \right] \quad , \quad (27)$$

where $I(t) = \exp(-\nu t) [\omega \sin(\omega t) - \nu \cos(\omega t)] + \nu$ and $A = \frac{a_o}{v^2 + \omega^2}$.

Equations (19), (25) and (27) have provided very useful checks on the computer code which incorporates a sinusoidally time-dependent external electric field. For example, Figs. 3 and 4 show a comparison of the time-dependence of the electron drift velocity and electron average energy, in a model gas with constant collision frequency and subjected to an external dc electric field, obtained from the numerical code and from the present analytical work [see Eqs. (20) and (25)]. Figs. 5 and 6 show a similar comparison for the case in which the external electric field is sinusoidally time-dependent with a frequency ω [see Eqs. (19) and (24)]. These comparisons have not only provided useful checks on the numerical results for electrons in real gases but have also enabled us to decide the actual time-step Δt and velocity step Δv which should be used for accurate numerical results, for both ac and dc electric fields. Eq. (27) can be used to understand, at least qualitatively, the conclusions reached from the results of Fig. 2.

1.5 Effect of the temperature of the background gas on $f(\mathbf{v}, t)$.

In the case where the background gas particles are at rest, even for *elastic* collisions of electrons (of mass m) with gas particles (of mass M) there is a transfer of energy, of the order of $\mu = m/M$, from the electron to the *recoiling* gas particle so that, in the absence of any external electric field, the numerical value of the average energy of electrons continues to reduce with time, approaching the unrealistic value of zero. A finite equilibrium value of the average electron energy is reached, numerically, only if one assumes $\mu = 0$. In order to make the situation in our calculations more realistic, we decided to investigate the effect of temperature (and, therefore, motion) of the background gas on the electron velocity distribution function. We assume that the number density of the gas particles is much larger than that of electrons so that electrons interact with gas particles more frequently than among themselves. Also, because of their large concentration, the gas particles interact with each other much more often than with electrons. Therefore, the background gas can be assumed to have a Maxwellian velocity distribution function, with a temperature parameter that varies slightly with time. The collision term, in general, has the form

$$R(\mathbf{v}, t) = \int \{f(\mathbf{v}', t) F(\mathbf{V}', t) - f(\mathbf{v}, t) F(\mathbf{V}, t)\} |\mathbf{v} - \mathbf{V}| \frac{d\sigma(\theta, \phi)}{d\Omega} d\Omega d\mathbf{V} \quad , \quad (28)$$

where \mathbf{v}' and \mathbf{V}' are the velocities of the electron and the gas particle before the collision and \mathbf{v} and \mathbf{V} are the corresponding velocities after the collision. $F(\mathbf{V}, t)$ is the Maxwellian velocity distribution function of the gas, $|\mathbf{v} - \mathbf{V}| = u$ is the relative velocity of the colliding partners and $\frac{d\sigma}{d\Omega}$ is the differential cross section for elastic scattering. In cylindrical coordinates the collision integral, for small but finite μ , can be written as

$$R(v_\rho, v_z, t) = \int_0^\pi \sin \psi d\psi \int_0^{2\pi} d\alpha \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \int_0^\infty \{f(v_\rho', v_z', t) F(V', t) u \frac{d\sigma}{d\Omega}\} V^2 dV - N \sigma_t f(v_\rho, v_z, t) v \quad (29)$$

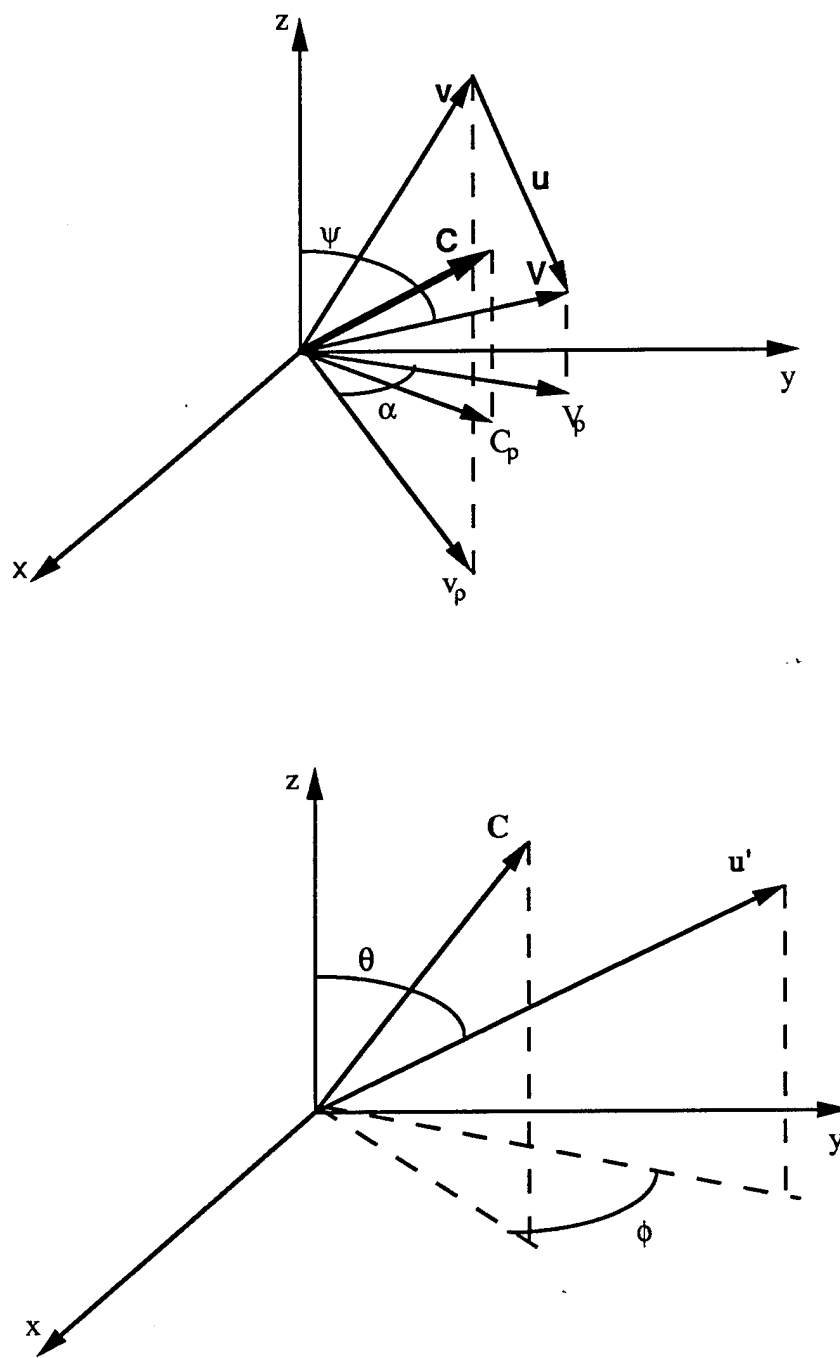


Fig. 7: Geometry of various vectors used in evaluating the collision integral.

where, as shown in fig. 7, ψ and α are the polar and azimuthal angles of \mathbf{V} , (θ, ϕ) are the scattering angles, σ_1 is the integrated elastic cross-section and N is the gas number density. The five-dimensional collision integral is evaluated, in the present work, numerically using the Monte Carlo technique. To do it we need to express v'_ρ , v'_z and V' in terms of v_ρ , v_z , V and all the relevant angles (ψ , α , θ and ϕ) using various conservation laws.

From the energy and momentum conservation laws we know that, in elastic collisions, the vector of center of mass velocity and the magnitude of relative velocity of the two colliding partners do not change. The center of mass velocity and relative velocity, given by

$$\mathbf{C} = \frac{m \mathbf{v} + M \mathbf{V}}{m + M} = \frac{m \mathbf{v}' + M \mathbf{V}'}{m + M}, \quad \mathbf{u} = \mathbf{V} - \mathbf{v}, \quad \mathbf{u}' = \mathbf{V}' - \mathbf{v}', \quad [\text{with } u = u']$$

have components

$$C_\rho = \frac{1}{1 + \mu} \sqrt{\mu^2 v_\rho^2 + V_\rho^2 + 2 \mu v_\rho V_\rho \cos \alpha}, \quad C_z = \frac{1}{1 + \mu} (\mu v_z + V_z),$$

$$u_\rho = \sqrt{v_\rho^2 + V_\rho^2 - 2 v_\rho V_\rho \cos \alpha}, \quad u_z = V_z - v_z, \quad \text{and} \quad u = \sqrt{u_\rho^2 + u_z^2}.$$

These relations provide the components of the center of mass velocity and the magnitude of relative velocity in terms of the velocities of particles after the collision. Now we need to obtain them in terms of the velocities before the collisions. Using

$$\mathbf{v}' = \mathbf{C} - \frac{1}{1 + \mu} \mathbf{u}',$$

the components of \mathbf{v}' and of \mathbf{u}' , in terms of scattering angles, are

$$v'_\rho = \sqrt{C_\rho^2 + \frac{1}{(1 + \mu)^2} u_\rho'^2 - \frac{2}{1 + \mu} u_\rho' C_\rho \cos \phi}, \quad v'_z = C_z - \frac{1}{1 + \mu} u_z',$$

$$\text{with } u_\rho' = u \sin \theta, \quad u_z' = u \cos \theta.$$

Various expressions, given above, combine together to provide the velocity of electron before the collision in terms of the required variables. Finally, we get V' using the energy conservation law:

$$V' = \sqrt{\mu (v^2 - v'^2) + V^2}.$$

Now we can carry out the five-dimensional integral using the standard Monte Carlo technique, that is, by generating random values of V , θ , ψ , ϕ , and α and by calculating the corresponding

integrand. Using this collision integral, which incorporates the effect of temperature of the background gas, in the Boltzmann equation we can evaluate the electron velocity distribution function. For this purpose, we investigated distribution of electrons in gaseous argon. The initial distribution of electrons is assumed to be a Maxwellian function, $f_{\text{Max}} \sim \exp(-v^2/v_{\text{th}}^2)$, where v_{th} is related to the electron temperature T_e (which is taken in this model investigation as 10^5 K) and the initial gas temperature is taken to be one-half of the electron temperature. For the mass ratio $\mu = 10^{-5}$, which is of correct order of magnitude for electrons in argon, fig. 8a compares the numerically calculated equilibrium electron velocity distribution function (solid line) with the initial Maxwellian distribution function (dashed line) for $v_p = 0$ and for no external electric field.

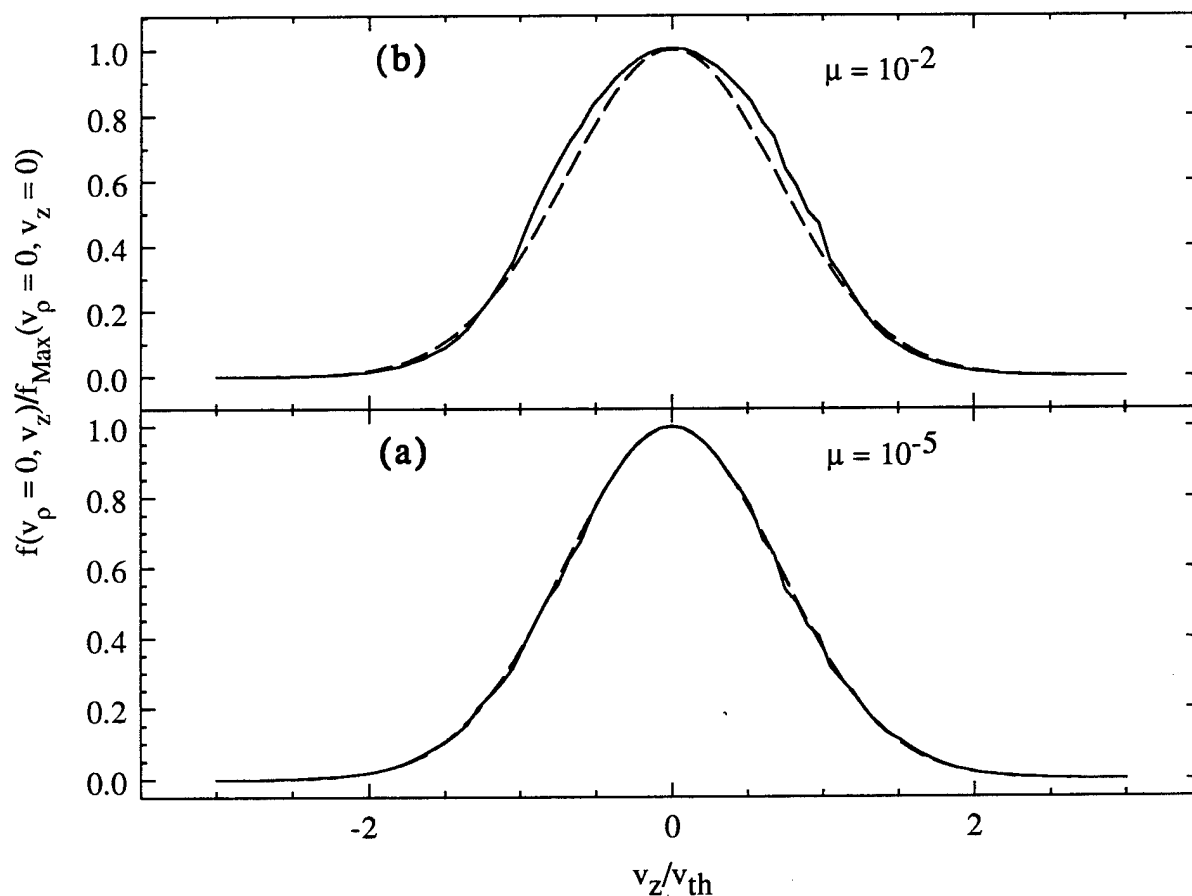


Fig. 8: Electron velocity distribution function for two different values of the mass ratio, μ .

Obviously, the effect of temperature of the ambient gas is hardly noticeable in this figure. However, if the magnitude of the mass ratio μ is artificially inflated to an unrealistic value of 10^{-2} , the electron velocity distribution function, at equilibrium, differs perceptibly, as seen in fig. 8b, from the initial Maxwellian function. Based on the results of fig. 8 it appears that the effect of temperature of the background gas on the electron velocity distribution function, and consequently on the swarm parameters, may not be important as long as there is no external electric field.

2. Comparative study of electron and positron transport in gases.

In order to compare the time-dependent behavior of a swarm of electrons in various atomic gases with the behavior of swarms of other charged projectiles, we have investigated the transport properties of electrons and positrons in the same ambient gas. Positrons, being antiparticles of electrons, are quite similar to electrons in all respects except that, unlike electrons, the polarity of their charge is positive. Investigations of the comparative behavior are accomplished by solving the Boltzmann transport equation exactly using our novel algorithm which has been described above. For both electrons and positrons, we have to include, in the collision term of the Boltzmann equation, the cross sections for the elastic, excitation and ionization processes. In addition, in the case of positrons, the effect of positronium formation and of positron annihilation had to be included to achieve the correct equilibrium values of various swarm parameters (such as the average energy and drift velocity of the projectiles as well as ionization and excitation rates of the background gas, etc.). The equilibrium values of the swarm parameters depend only on the ratio E/N , the ratio of the applied external electric field to the gas number density. In order to assess the accuracy of the present numerical results in the comparative study, we first calculated drift velocity of electrons in pure gaseous neon for which considerable experimental data is available for comparison. Fig. 9 shows the drift velocity of electrons in neon for several values of E/N and it seems to agree quite favorably with the corresponding experimental data of Pack [3], Robertson [4] and Nielson [5]. This superb agreement provides confidence in the accuracy of our

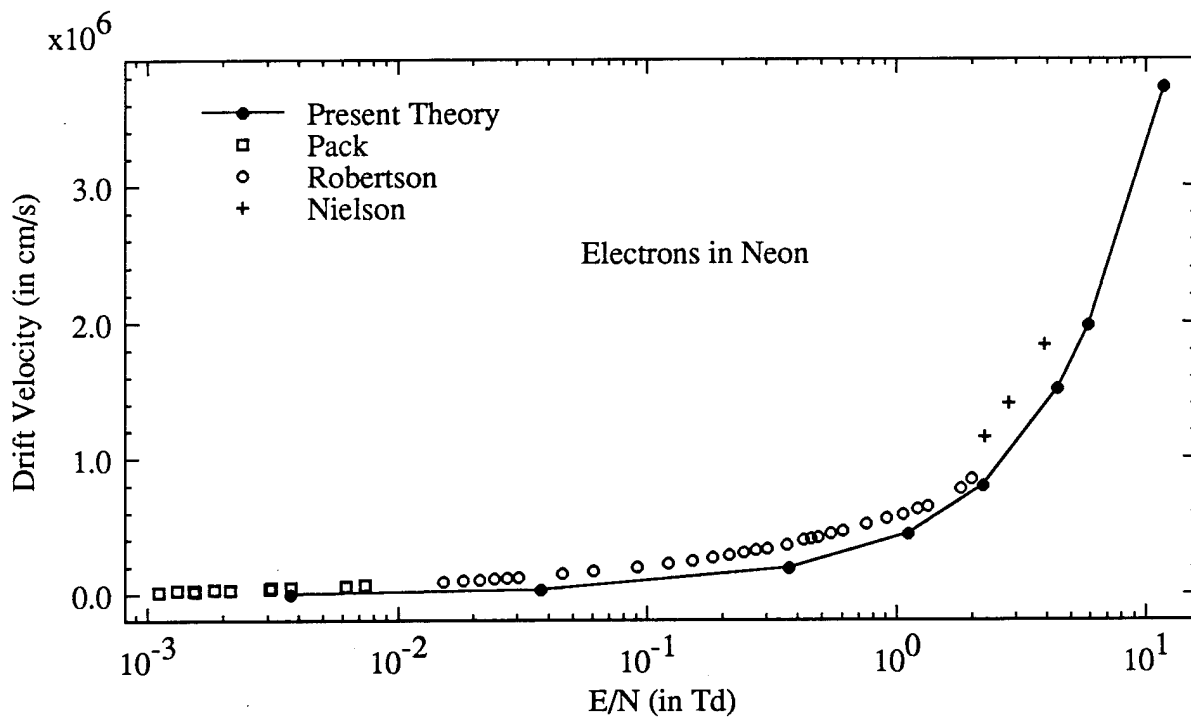


Fig. 9: A comparison of the present values of the drift velocity of electrons in neon as a function of E/N with the corresponding experimental values.

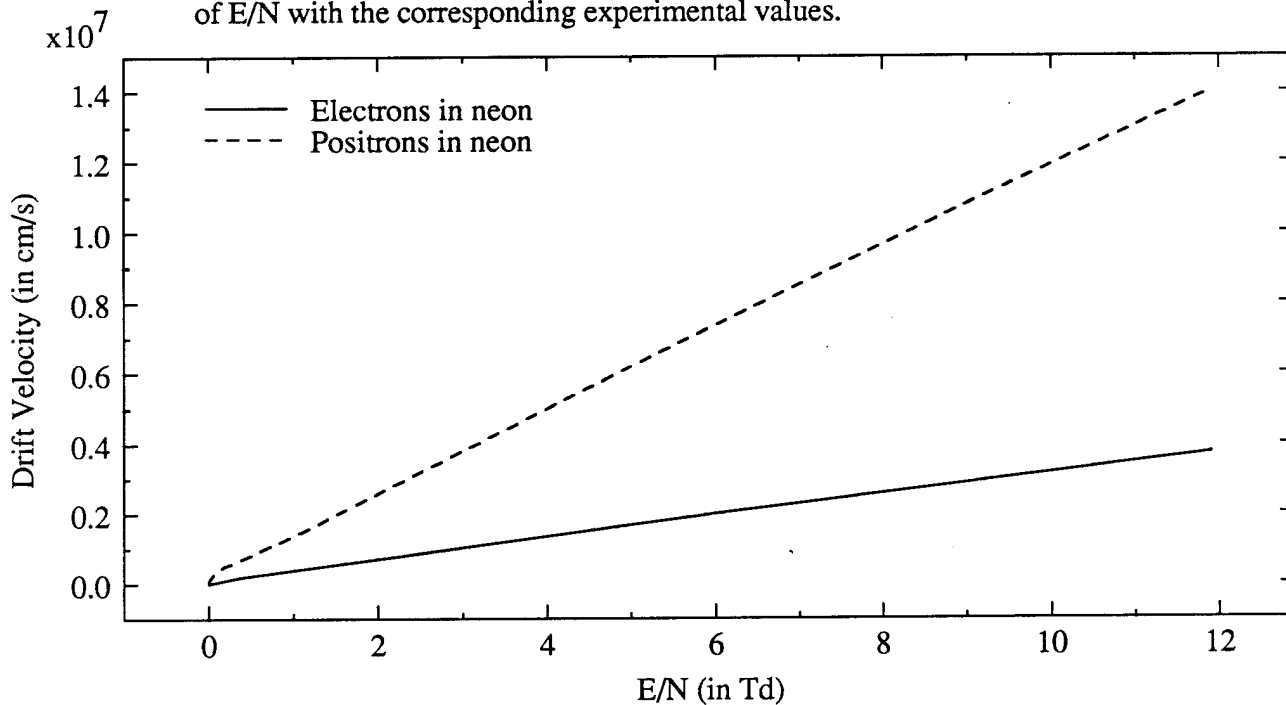


Fig. 10: Drift velocity of electrons and of positrons as a function of E/N in gaseous neon.

numerical results for various swarm parameters. Now, for the comparative study, Fig. 10 displays, as an example, the equilibrium values of the drift velocity of electrons and of positrons in the same gas (namely, neon) for the same values of E/N . As expected, the drift velocity for both projectiles approaches zero as $E/N \rightarrow 0$. However, for higher values of E/N , the drift velocity (and, therefore, mobility) of positrons is consistently larger, by almost a factor of 2.5, than the drift velocity of electrons in neon. It is anticipated that investigations of transport properties of several different projectiles in the same gas will assist in optimizing the choice of the projectile to be used in the gas for the particular application at hand.

3. Dissociation of vibrationally excited H_2 by electron impact

As part of our investigations we have continued to calculate the cross sections for the processes which are important for a realistic modeling of the hydrogen plasma. In a typical hydrogen source, vibrationally excited H_2 molecules are depleted both by dissociative electron attachment and by pure dissociation of the molecule. Since previous investigations have clearly demonstrated that the cross sections for dissociative electron attachment to H_2 are significantly enhanced if the molecule H_2 is initially vibrationally excited, it is, then, natural to ask whether the cross sections for pure dissociation of H_2 are also strongly dependent upon the initial vibrational state of H_2 . In the present investigations we have interpreted the process of pure dissociation of H_2 as an extension of the process of vibrational excitation of H_2 by electron impact in which the final vibrational level lies in the continuum. In such a situation the dissociation of the molecule will occur, analogous to the vibrational excitation of molecule, predominantly via the formation of an electron-molecule resonance. The significance of a resonance formation for the vibrational excitation to occur can be appreciated by a simple analogy: A small bee kicking (or colliding with) a large elephant would not cause much perturbation to the elephant unless it stays and buzzes around the big animal for a time period much longer than the normal transit flying time of the bee. During a collision it will be easier for an electron to change the vibrational mode of a much more massive molecule if it can form a resonance with the molecule. At low energies electron can form

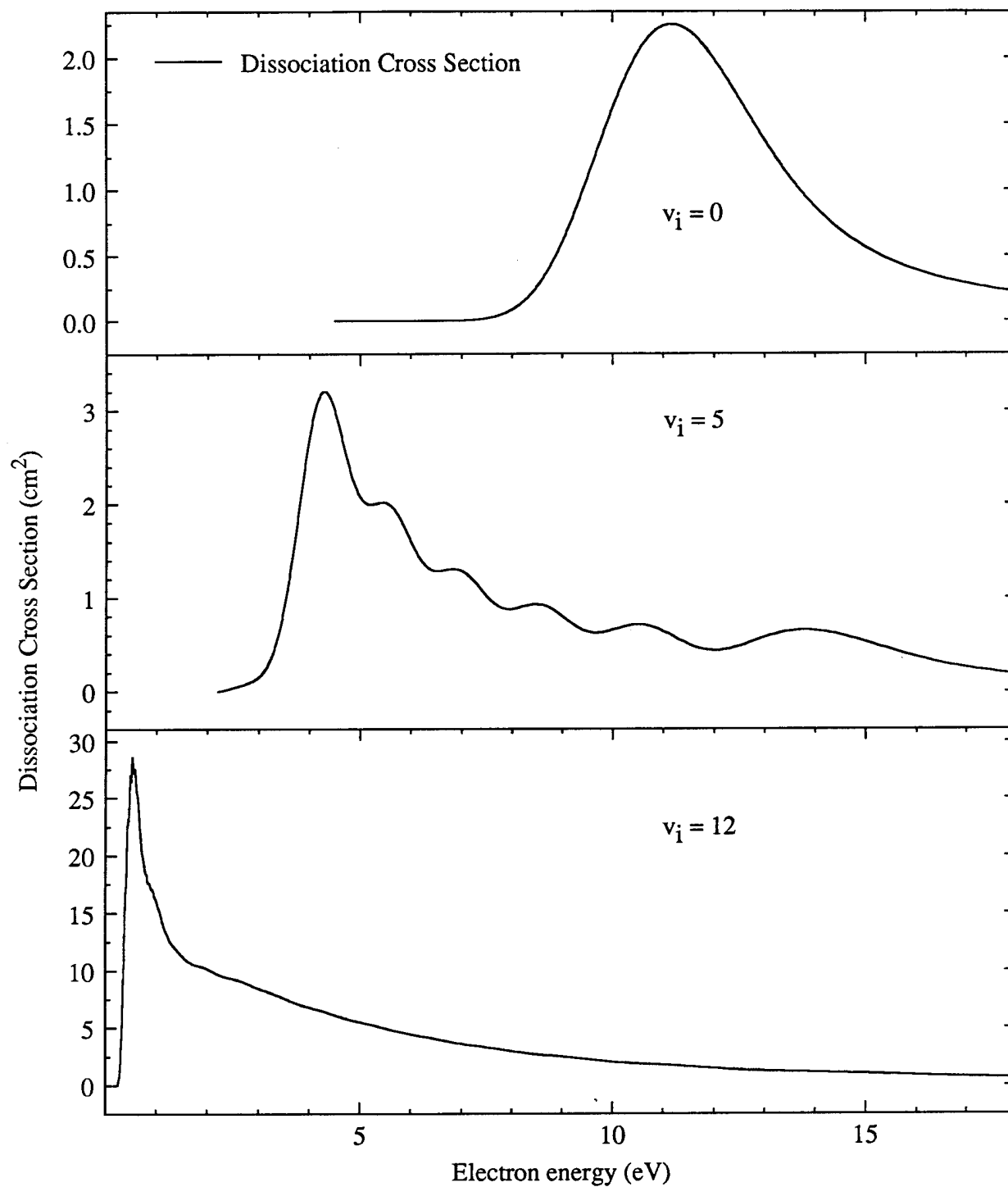
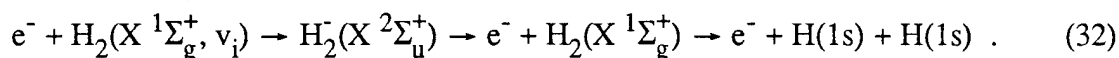
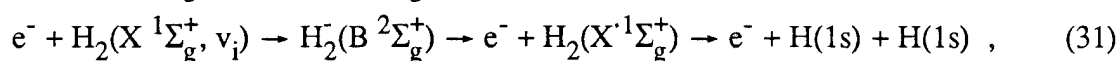
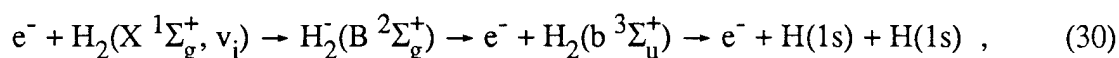


Fig. 11: Total cross sections for the electron impact dissociation of vibrationally excited H₂. v_i is the initial vibrational quantum number of the molecule H₂.

two distinct resonances with H_2 molecule; these two resonant states of H_2^- are the $X^2\Sigma_u^+$ and $B^2\Sigma_g^+$ states. The $X^2\Sigma_u^+$ resonance decays only to the ground electronic state, $X^1\Sigma_g^+$, of molecular hydrogen while the $B^2\Sigma_g^+$ resonance can, over a certain range of internuclear separations, decay both to the excited $b^3\Sigma_u^+$ state and the ground $X^1\Sigma_g^+$ state of H_2 . Thus, in our calculations, we have included the following three channels:



Using the traditional formalism of the resonance theory, we have calculated the sum of the cross sections for the dissociation of H_2 by low energy electron impact via each of these three channels (Eqs. (30-32)). The total dissociation cross sections of H_2 in various initial vibrational levels v_i are shown in fig. 11. For any initial vibrational levels v_i the contribution of channel (31) is negligible at all electron energies while channel (30) contributes significantly at all energies where this channel is energetically open. Contribution of channel (32), on the other hand, is insignificant for low values of v_i but increases dramatically as v_i is increased and for large initial vibrational excitation of the molecule ($v_i \geq 8$) the contribution of channel (32) can become comparable to the contribution of channel (30). The details of this work have been published as a letter in a refereed journal [6].

4. Asymptotic form of the penetration probability of the quantum harmonic oscillator into the classically forbidden region

During the course of present investigations, we came across an interesting problem that apparently has not been addressed in any previously published work. The problem concerns a linear harmonic oscillator of which both the classical and the quantum versions have been studied quite extensively. Surprisingly, however, little seems to be known about the quantum-mechanical probability $P(n)$ of finding the oscillator outside the classical turning points when the quantum

number n is large, notwithstanding the obvious expectation, based on the correspondence principle, that this probability must somehow tend to zero as the quantum number tends to infinity. A recent article [7] presented a conjecture, supported by a *purely numerical* investigation, that this probability has the asymptotic form

$$P(n) = A \left(n + \frac{1}{2} \right)^{-1/3} - B \left(n + \frac{1}{2} \right)^{-1} + \dots \quad (33)$$

as $n \rightarrow \infty$, with $A \approx 0.133970$ and $B \approx 0.011907$. The main purpose of our work was to derive an asymptotic formula for this penetration probability using an *analytic* argument based on the behavior of the harmonic oscillator eigenfunctions in the vicinity of the classical turning points for large quantum numbers. We have shown that this analytical result is identical in form to Eq. (33). We have derived closed-form expressions for the coefficients A and B , and their values are found to be quite close to those quoted above. The derivation has also yielded the order of the first neglected term. As a further demonstration of the usefulness of the asymptotic forms of the harmonic oscillator eigenfunctions, a formula for the quantum probability density *inside* the classical turning points in the large- n limit is briefly derived and is seen to have a simple physical interpretation.

The energy eigenstate of the quantum harmonic oscillator corresponding to the quantum number n has energy $E_n = \left(n + \frac{1}{2} \right) \hbar \omega$ relative to the potential minimum, and the corresponding normalized eigenfunction is given by

$$\psi_n(x) = (2^n n! \sqrt{\pi} x_0)^{-1/2} \exp(-x^2/2x_0^2) H_n(x/x_0)$$

where the H_n are the Hermite polynomials, and $x_0 = \sqrt{\frac{\hbar}{m\omega}}$. The classical turning points occur at

$$x = \pm \sqrt{2v} x_0$$

where for convenience, both here and later, we put $v \equiv n + 1/2$. The probability of finding the oscillator outside the classical turning points is therefore

$$P(n) = 2 \int_{\sqrt{2\nu} x_0}^{\infty} dx |\psi_n(x)|^2 = 2 (2^n n! \sqrt{\pi} x_0)^{-1} \int_{\sqrt{2\nu} x_0}^{\infty} dx \exp(-x^2/x_0^2) [H_n(x/x_0)]^2$$

or, changing the variable of integration from x to $y = x/x_0$,

$$P(n) = \frac{1}{2^n n!} \frac{2}{\sqrt{\pi}} \int_{\sqrt{2\nu}}^{\infty} dy \exp(-y^2) [H_n(y)]^2 \quad (34)$$

Now, using the asymptotic properties of the Hermite polynomials we have shown that $P(n)$ can be expressed as

$$P(n) \approx 2I_1 \nu^{-1/3} - \left(\frac{4}{5} I_3 + \frac{6}{5} I_2\right) \nu^{-1} + O(\nu^{-5/3}) \quad (35)$$

with

$$I_1 = \int_0^{\infty} dx \text{Ai}^2(x) = \frac{3^{1/3}}{4 \pi^2} \left[\Gamma\left(\frac{2}{3}\right) \right]^2,$$

$$I_2 = \int_0^{\infty} dx x \text{Ai}^2(x) = \frac{1}{6 \pi \sqrt{3}}$$

$$I_3 = \int_0^{\infty} dx x^2 \text{Ai}'(x) \text{Ai}(x) = - \int_0^{\infty} dx x \text{Ai}^2(x) = -I_2$$

where $\text{Ai}(x)$ is the standard Airy's function which is related to the modified Bessel function as

$$\text{Ai}(x) = \frac{1}{\pi} \sqrt{\frac{x}{3}} K_{1/3} \left(\frac{2}{3} x^{3/2} \right)$$

The integrals I_1 and I_2 are easily evaluated using the standard integral [8],

$$\int_0^{\infty} dx x^{\alpha-1} K_{\mu}^2(x) = \frac{2^{\alpha-3}}{\Gamma(\alpha)} \Gamma\left(\frac{\alpha}{2} + \mu\right) \Gamma\left(\frac{\alpha}{2} - \mu\right) \left[\Gamma\left(\frac{\alpha}{2}\right) \right]^2.$$

The asymptotic form of the penetration probability is thus found to be approximately

$$P(n) \approx A (n + 1/2)^{-1/3} - B (n + 1/2)^{-1} + O\left((n + 1/2)^{-5/3}\right)$$

with

$$A = \frac{3^{1/3}}{2 \pi^2} \left[\Gamma\left(\frac{2}{3}\right) \right]^2 \approx 0.133975, \quad B = \frac{1}{15 \pi \sqrt{3}} \approx 0.012252 \quad (36)$$

in good agreement with the values quoted above in the introductory paragraph, which were obtained by purely numerical methods [7].

It is of interest to examine the absolute error in the first two terms of Eq. (33). Denote this quantity as $\delta(n)$, i.e., define

$$\delta(n) = P(n) - A(n + 1/2)^{-1/3} + B(n + 1/2)^{-1}$$

In fig. 12 the absolute error $\delta(n)$ is plotted against $(n + 1/2)^{-5/3}$ for $n = 50, 60, 70, \dots, 350, 400, 500$ using the coefficients A and B given by Eq. (36). The values of $P(n)$ were obtained by numerical integration of the right-hand side of Eq. (34) with respect to y^2 , using Simpson's rule, on a grid of step size 0.01, in REAL*8 precision on a SGI Iris Indigo computer. The solid line in the figure is the best linear fit through all the points. It is noteworthy that all of the values of $\delta(n)$ lie very nearly on this line, a fact which is consistent with the O-term in Eq. (35).

It is also interesting to consider the probability density in the state ψ_n inside the classical turning points. In elementary textbooks on quantum mechanics [9, 10] one often sees plots like the one in fig. 13, showing, for some large value of n (in this case $n = 50$), the probability density as calculated from quantum mechanics, compared with the corresponding *classical* probability density

$$P_{cl}(x) = \pi^{-1} (2v x_0^2 - x^2)^{-1/2}$$

for a harmonic oscillator of the same energy. The classical probability density is easily derived by considering the fraction of time the oscillator spends in the interval between x and $x + dx$; that fraction is just $P_{cl}(x) dx$. Intuitively one sees that the "envelope" of the quantum curve follows the classical curve more and more closely as n increases. This can be seen analytically as well; yet this fact is not shown in any textbook or paper of which we are aware. Using an asymptotic series which describes the behavior of the Hermite polynomials for large order we have shown that

$$|\psi_n(x)|^2 \approx P_{cl}(x) \left\{ 2 \sin^2 \left[v \left(\theta - \frac{1}{2} \sin 2\theta \right) + \frac{\pi}{4} \right] + O(v^{-1}) \right\},$$

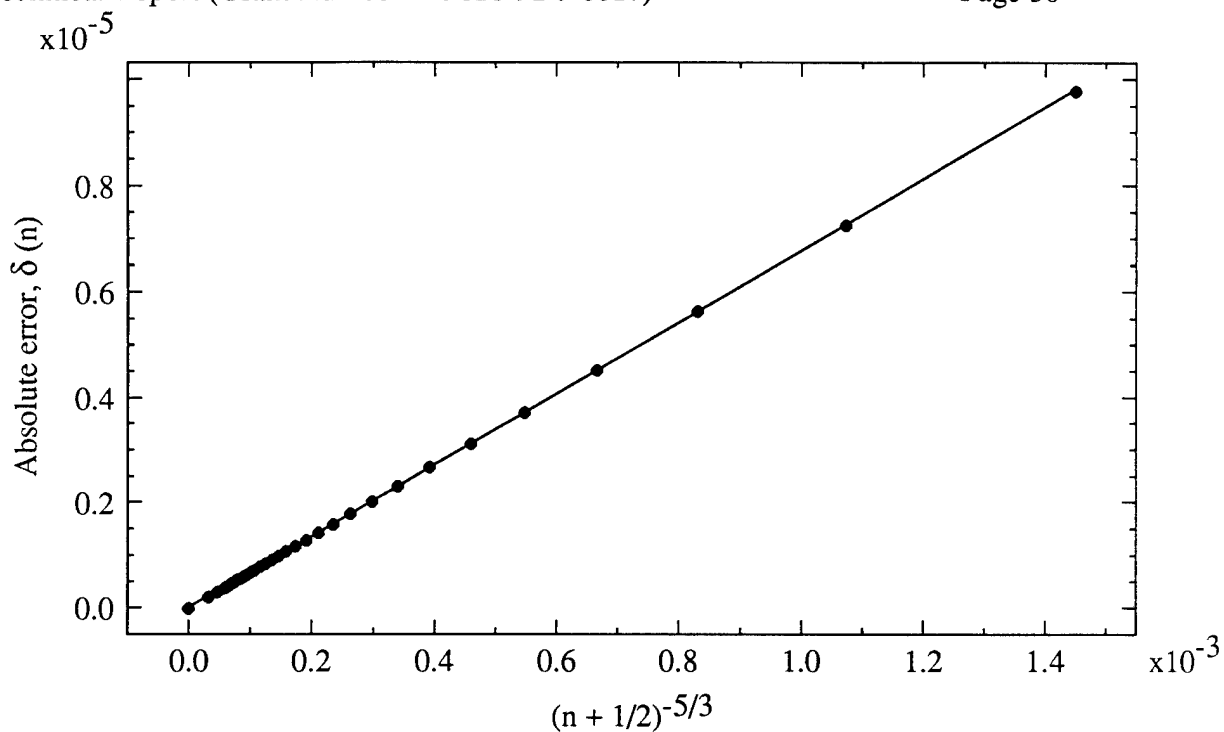


Fig. 12: The absolute error $\delta(n)$ for $n = 50, 60, 70, \dots, 350, 400, 500$, and the best straight line fit through all the points.

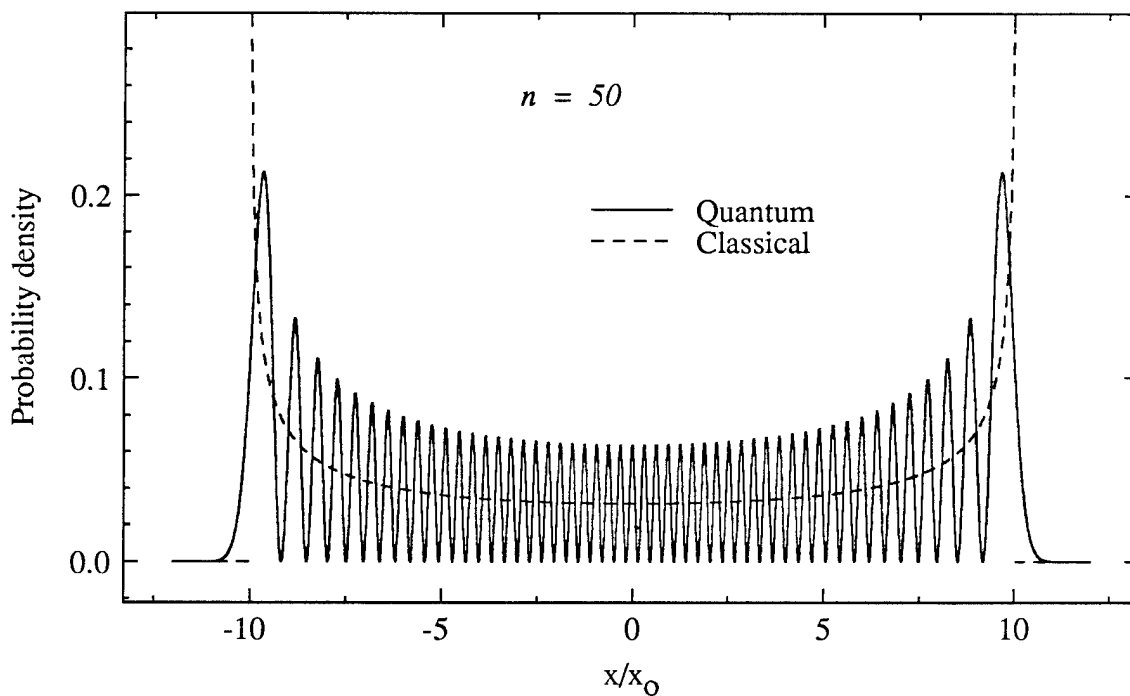


Fig. 13: The dimensionless probability density $x_0 |\psi_n(x)|^2$ of a quantum oscillator for $n=50$ and the corresponding probability density $\pi^{-1} (2v - x^2/x_0^2)^{-1/2}$ for a classical oscillator of the same energy.

as $n \rightarrow \infty$. Thus to leading order, the quantum probability density inside the classical turning points is indeed, for large quantum numbers, a rapidly oscillating function modulated by a more slowly varying "envelope" consisting of its classical counterpart.

In conclusion, we have analytically derived an asymptotic formula for the penetration probability of the quantum harmonic oscillator into the classically forbidden region for large quantum numbers, and seen that it is in reasonably good agreement with an asymptotic formula obtained previously [7] by numerical methods. We have also used a numerical calculation to support the derived order of the error in the first two terms of this formula. Finally, we have shown that the leading-order term in the asymptotic expansion, for large quantum numbers, of the quantum probability density inside the classical turning points has a form which is readily understood physically in light of the correspondence principle. The details of the analytical work are in our paper which has appeared in the American Journal of Physics [11].

5. Presentations / Publications

During the tenure of the present Grant we have made presentations of our research investigations at various national and international scientific conferences. These are

- "Time-dependence of swarm parameters of electrons in argon", (with A. A. Sebastian); presented at the 44th Annual Gaseous Electronics Conference, Albuquerque, New Mexico, October 22-25, 1991.
- "The mass dependence of cross sections for vibrational excitation of diatomic molecules by electron impact", (with D. E. Atems); presented at the 44th Annual Gaseous Electronics Conference, Albuquerque, New Mexico, October 22-25, 1991.
- "A new isotope scaling law for vibrational excitation of diatomic molecules by electron impact", Bull. Am Phys. Soc. 37, 1093 (1992) (with D. E. Atems); presented at the 1992 Annual Meeting of the Division of Atomic, Molecular and Optical Physics, Chicago, Illinois, May 19-22, 1992.

- "Electron transport in argon and neon under the influence of an rf electric field", Bull. Am Phys. Soc. 37, 1114 (1992) (with A. A. Sebastian and P. J. Drallos); presented at the 1992 Annual Meeting of the Division of Atomic, Molecular and Optical Physics, Chicago, Illinois, May 19-22, 1992.
- "Transport of electrons in hydrocarbon gases at high E/N", (with A. A. Sebastian and P. J. Drallos); presented at the 45th Annual Gaseous Electronics Conference, Boston, Massachusetts, October 27-30, 1992.
- "Effect of an rf electric field on the charged particle transport in rare gases", Bull. Am. Phys. Soc. 37, 1544 (1992) (with A. A. Sebastian); presented at the Thirty-Fourth Annual Meeting of the Division of Plasma Physics, Seattle, Washington, November 16-20, 1992.
- "Transport of electrons in simple hydrocarbon gases subjected to external electric fields", (with A. A. Sebastian); presented at the Eighteenth International Conference on the Physics of Electronic and Atomic Collisions, Aarhus, Denmark, July 21-27, 1993.
- "Effect of initial vibrational excitation on the dissociation of H₂ by low-energy electron impact", (with D. E. Atems); presented at the Eighteenth International Conference on the Physics of Electronic and Atomic Collisions, Aarhus, Denmark, July 21-27, 1993.
- "Electron transport in hydrocarbon-rare gas mixtures", (with A. A. Sebastian); presented at the 46th Annual Gaseous Electronics Conference, Montreal, Quebec, October 19-22, 1993.
- "Charged particle transport in mixtures of hydrocarbon and rare gases subjected to external fields", Bull. Am. Phys. Soc. 38, 1994 (1993) (with A. A. Sebastian); presented at the Thirty-Fifth Annual Meeting of the Division of Plasma Physics, St. Louis, Missouri, November 1-5, 1993.
- "Electron transport in mixtures of hydrocarbon and rare gases subjected to a time-dependent rf electric field", (with A. A. Sebastian); presented at the 1994 Annual Meeting of the Division of Atomic, Molecular and Optical Physics, Washington, DC, April 18-21, 1994.

During the tenure of the present Grant, our research investigations have led to the following

refereed publications:

- "Vibrational excitation of H₂ and HCl by low-energy electron impact: An isotope scaling law", *D. E. Atems and J. M. Wadehra*, Chem. Phys. Letts. 197, 525 (1992).
- "A new representation of the generalized oscillator strength for bound - free transitions in hydrogenlike systems", *J. M. Wadehra and S. P. Khare*, Phys. Letts. A172, 433 (1993).
- "Resonant contributions to dissociation of H₂ by low-energy electron impact", *D. E. Atems and J. M. Wadehra*, J. Phys. B Letter 26, L759 (1993).
- "Asymptotic form of the penetration probability of the quantum harmonic oscillator into the classically forbidden region", *D. E. Atems and J. M. Wadehra*, Am. J. Phys. 63, 443 (1995).
- "Electron attachment to molecules at low electron energies", *A. Chutjian, A. Garscadden and J. M. Wadehra*, Phys. Rep. (accepted, 1995).

In addition, the following papers are under preparation and will be submitted to refereed journals for publication soon:

- "Exact numerical solutions of the Boltzmann equation for electrons in gases subjected to external electric fields", *A. A. Sebastian and J. M. Wadehra*, (1996).
- "Exactly solvable model for the time-dependence of charged particle swarms in gases subjected to external fields", *A. A. Sebastian and J. M. Wadehra*, (1996).

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