Diffusion of electrons in a gas in the field of an intense coherent radiation

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A theory of electron diffusion in a gas in the presence of an intense radiation field is presented. The theory is applicable when the classical electron oscillation energy ϵ_0 exceeds the typical electron-gas inelastic collision energy loss ξ and when the frequency ω of the wave is much larger than the inelastic collision frequency $\nu_{\rm coll}$. It is shown that the existence of these two different time scales allows us to derive a simple Langevin type, model stochastic equation, describing the slow-time-scale electron transport in the gas. Assuming linear dependence of $\nu_{\rm coll}$ on the electron energy, simple analytic expressions for the time evolution of the average electron translational energy W and random-walk parameter $\langle x^2\rangle_{\rm av}$ are derived. In the long-time limit $W=\xi/4$ and $\langle x^2\rangle_{\rm av}=Dt$, where the diffusion coefficient D is independent of both ω and ϵ_0. These predictions are in a good agreement with the results of Monte Carlo computer experiments, conducted for the cases of N_2 and Hg.

I. INTRODUCTION

Self-consistent theoretical determination of electron diffusion coefficient in a gas in the presence of an electromagnetic wave usually requires a solution of the Boltzmann equation.[1] This can be conveniently accomplished in the case when the electromagnetic field is so weak that the classical electron oscillation energy $\epsilon_0=e^2E^2/2m\omega^2$ (E and ω being the amplitude and frequency of the electric field of the wave) is much less than the average energy $\bar{\epsilon}$ of the electrons. Such a situation exists, as a rule, when $\xi_{\rm el}\ll\epsilon_0\ll\xi_{\rm in}$, where $\xi_{\rm in}$ and $\xi_{\rm el}\simeq 2\bar{\epsilon}m/M$ are the characteristic electron-energy losses in inelastic and elastic collisions, respectively. Indeed, in this case, the electrons gain the translational energy via the inverse bremsstrahlung, until the energy growth saturates due to the inelastic collisions and a steady state is achieved in which $\bar{\epsilon}$ is of the order of $\xi_{\rm in}$, or more, and therefore $\bar{\epsilon}\gg\epsilon_0$. Then the smallness of the oscillating component of the velocity, allows us to seek a solution of the Boltzmann equation in the form of the two-term Lorentz equation[2] $f(\mathbf{v},t)=f_0(\mathbf{v})+f_1(\mathbf{v},t)$, where formally $|f_1|/|f_0|\ll 1$ and therefore a perturbation method can be applied in solving for f_0 and f_1. The time-independent part f_0 of the distribution usually serves to calculate the diffusion coefficient, while the small oscillatory part f_1 describes the polarization current.

In the present work we will consider a different situation of radiation fields so intense that the aforementioned perturbative procedure cannot be applied. This usually happens when $\epsilon_0>\xi_{\rm in}$ and the characteristic electron-gas collision frequency $\nu_{\rm coll}$ is much smaller than ω.

In this case the velocity of the electrons oscillates with large amplitude $a=(2\epsilon_0/m)^{1/2}$ many times between successive collisions. The translational component of the velocity, in contrast, remains relatively small because the inverse bremmstrahlung type heating of the electrons at $\epsilon>\xi_{\rm in}$ is negligible compared to the energy losses in inelastic collisions. Thus, in the case considered here $\bar{\epsilon}\simeq\epsilon_0$, in contrast to a typical weak radiation-field case. Situations which fall into such intense-field regime can be found in various applications. For example, for the radiation flux of ~ 0.5 MW/cm^2 and $\omega=30$ GHz we have $\epsilon_0\simeq 10$ eV. Thus, assuming that typically $\nu_{\rm coll}\simeq 10^9$ (sec Torr)$^{-1}$, the intense-field conditions in this case exist at pressures lower than 20 Torr. Therefore, the present theory may be of interest in projected electron cyclotron resonance heating experiments in large laboratory plasmas.[3] Similar parameter regime characterizes gas breakdown by intense picosecond Nd glass-laser pulses.[4] Here $\epsilon_0>10$ eV for fluxes of more than 5×10^{13} W/cm^2, while $\omega\gg\nu_{\rm coll}$ at $p\lesssim 100$ atm.

In the following theory we will concentrate on a single-electron diffusion process. It should be mentioned, however, that since $\epsilon_0>\xi_{\rm in}$, the diffusion is also accompanied by a rapid electron multiplication due to ionizing collisions. The theory of the current growth in such a highly nonlocal and time-dependent situation is out of the scope of the present work and will be described elsewhere.[5]

The content of the paper will be as follows. In Sec. II we will derive and solve a model stochastic equation, describing the electron transport. Section III will describe a Monte Carlo computer experiment for testing the theory. Finally, in Sec. IV we will discuss the results of the simulations as well as the limitations of the proposed theoretical model.

II. MODEL STOCHASTIC EQUATION

Consider an electron in a gas in the presence of the electric field of the form

$$\mathbf{E}(t)=\mathbf{E}_0\cos(\omega t),\quad \mathbf{E}_0=\text{const}\ . \tag{1}$$

We are interested in the nonrelativistic case ($v/c\ll 1$) and therefore, in studying the electron motion, neglect the magnetic component of the electromagnetic wave, as well as the dependence of $\mathbf{E}$ on position. Assume that E_0 is large enough so that in collisions with the gas molecules, the electron is scattered mainly in the forward direction. Consequently, for simplicity, we are adopting a one-

dimensional scattering model, in which only inelastic collisions influence the motion of the electron.

Chose the x axis in the direction of $\mathbf{E}_0$ and assume that at $t=t_0$ the electron is at rest. Then, if the first inelastic collision occurs at $t=t_1$, the velocity of the electron for t in the interval (t_0,t_1) will be

$$v_0(t)=-a[\sin(\omega t)-\sin(\omega t_0)] , \tag{2}$$

where $a=eE_0/m\omega=(2\epsilon_0/m)^{1/2}$. Similarly, the velocity between the first and the second inelastic collisions is

$$v_1(t)=\Delta_1-a[\sin(\omega t)-\sin(\omega t_0)] , \tag{3}$$

where Δ_1 is the change in the velocity in the first collision. More generally, between the nth and $(n+1)$th collisions $(t_n<t<t_{n+1})$,

$$v_n(t)=V_n-a\sin(\omega t) , \tag{4}$$

where

$$V_n=a\sin(\omega t_0)+\sum_{i=1}^{n}\Delta_i \tag{5}$$

is the translational part of the velocity which, obviously, leads to the electron transport in the gas. In order to understand how V_n evolves in time, consider the three possibilities shown schematically in Fig. 1, where we see the velocity $v(t)$ for three different domains of V. Using the fact that the sign of Δ_{n+1} (which describes the direction of the change of V_n) is opposite to the sign of $v_n(t)$ at the moment of the $(n+1)$st collision, we conclude that in the case in Fig. 1(a), where $V_n>a/2$, most probably V_{n+1} is less than V_n. Similarly, for $V_n<-a/2$ [Fig. 1(b)], most probably $\Delta_{n+1}>0$, so that $V_{n+1}=V_n+\Delta_{n+1}>V_n$. Thus, for $|V_n|>a/2$, on the coarse-time scale when the fast oscillations are averaged out (note that we assume $\omega\gg\nu_{\text{coll}}$), we can attempt to describe the evolution of V_n by the dynamic friction-type equation

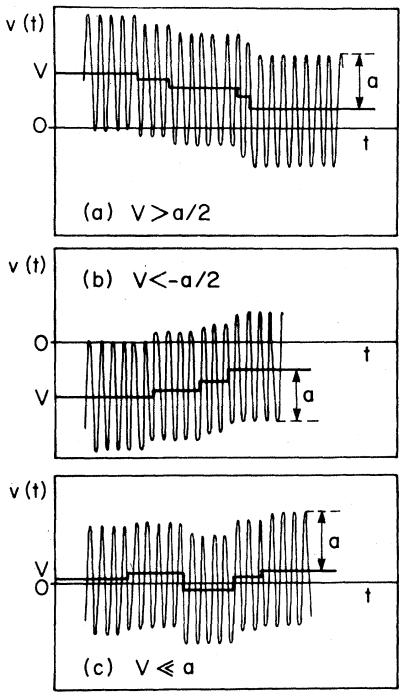

FIG. 1. Dependence of the electron velocity v on time. (a) and (b) Large translational velocity V ($|V|>a/2$). The graduate decrease of $|V|$ is characteristic in this case. (c) $|V|\ll a$. The translational component of the velocity changes rather randomly in collisions.

$$\frac{dV}{dt}=-\beta V . \tag{6}$$

In order to find the friction coefficient β in (6), assume the following simple dependence of the inelastic collision frequency on the electron energy ϵ:

$$\nu_{\text{coll}}=pk\epsilon , \tag{7}$$

where $k=$const and p is the pressure of the gas. Assume also that in every inelastic collision the electron loses the same amount of energy ξ and that $\xi\ll\epsilon_0$. Then, most probably, the electron energy ϵ in collisions will be also much larger than ξ, so that approximately $m|\Delta||v|=\xi$, or

$$|\Delta|\simeq\xi/(2m\epsilon)^{1/2} . \tag{8}$$

Therefore, we find

$$\beta\simeq\frac{|\Delta|}{|v|}\nu_{\text{coll}}\simeq\frac{pk\xi}{2} . \tag{9}$$

Equation (6) predicts a continuous exponential decrease of $|V|$ on the coarse-time scale. As was demonstrated earlier, such a *deterministic* friction effect is dominant at $|V|>a/2$. For $|V|<a/2$ and especially when $|V|\ll a$, in addition to the friction, we find rather random changes of both the sign and the magnitude of V. In fact, as can be seen in Fig. 1(c), if $|V|\ll a$, the oscillating electron spends almost equal amount of time in negative and positive regions of $v_n(t)$, so that with almost equal probability, Δ_{n+1} can be positive or negative. Thus, in this regime (in which also $\beta V\simeq 0$), the coarse-time evolution of V can be described by a stochastic equation of the form

$$\frac{dV}{dt}=A(t) , \tag{10}$$

where $A(t)$ is a random function of t with zero average over an ensemble of realizations:

$$\langle A(t)\rangle_{\text{av}}=0 . \tag{11}$$

We also assume that $A(t)$ is only correlated with itself over an average time between collisions,

$$\tau=1/\langle\nu_{\text{coll}}\rangle_{\text{av}}\simeq 2/pk\epsilon_0=4/pkma^2 . \tag{12}$$

We furthermore assume that $A(t)$ describes a stationary process so that the correlation function $\langle A(t')A(t'')\rangle_{\text{av}}$ depends only on the difference $t'-t''$. Then [see (8)]

$$\langle|\Delta|\rangle_{\text{av}}\simeq\sqrt{2}\xi/ma=\bar{\Delta} , \tag{13}$$

and we can approximately estimate the integral

$$I=\int_{-\infty}^{+\infty}\langle A(0)A(t)\rangle_{\text{av}}dt\simeq\frac{\bar{\Delta}^2}{\tau}=\xi^2pk/2m . \tag{14}$$

Equations (6) and (10) describe the coarse-time evolution of V in the complementary domains of large or small values of V, respectively. The two different effects described by these equations can thus be also represented by a single Langevin equation

$$\frac{dV}{dt}=-\beta V+A(t) . \tag{15}$$

This is the desired model stochastic equations, describing the electron transport in our problem. Note that the rapid-time variation, due to the high frequency ω of the electromagnetic wave, had been factored out in (15) which is a direct consequence of our assumption of $\omega \gg \nu_{\text{coll}}$.

We now formally solve (15), assuming that $V(0)=a\sin(\omega t_0)$ [see Eq. (5)],

$$V(t)=a\sin(\omega t_0)e^{-\beta t}+e^{-\beta t}\int_0^t dt'\,A(t')e^{\beta t'} . \tag{16}$$

Obviously $\langle V(t)\rangle_{\text{av}}=0$. Next, we square (16) and ensemble average

$$W=\frac{m}{2}\langle V^2(t)\rangle_{\text{av}} = \frac{\epsilon_0}{2}e^{-2\beta t} + \frac{m}{2}e^{-2\beta t}\int_0^t dt'\,e^{\beta t'}\int_0^t dt''\,e^{\beta t''}\langle A(t')A(t'')\rangle_{\text{av}} . \tag{17}$$

Equation (17) can be further simplified if we use the fact that as long as $\epsilon_0 \gg \xi$, the autocorrelation time τ of $A(t)$ is much less than the relaxation time $1/\beta$ [see Eqs. (9) and (12)]. This allows on even coarser scale (namely for $t \gg \tau$) to replace $e^{\beta t''}$ in (17) by $e^{\beta t'}$ and the limits in the second integral by $\pm\infty$. This yields

$$W=\frac{\epsilon_0}{2}e^{-2\beta t}+\frac{m}{4\beta}(1-e^{-2\beta t})I \tag{18}$$

or, on using (14) and (9),

$$W=\left[\frac{\epsilon_0}{2}-\frac{\xi}{4}\right]e^{-2\beta t}+\frac{\xi}{4} . \tag{19}$$

Thus $\lim_{t\to\infty} W=\xi/4$.

Velocity (16) can now serve to find electron diffusion coefficient. The coarse-time ($t \gg 1/\omega$) evolution of the coordinate of the electron is given by

$$x(t)=\int_0^t V(t')dt' = \frac{a\sin(\omega t_0)}{\beta}(1-e^{-\beta t}) + \int_0^t dt'\,e^{-\beta t'}\int_0^{t'} dt''\,A(t'')e^{\beta t''} \tag{20}$$

or, on taking the double integral in (20) by parts,

$$x(t)=\frac{1}{\beta}a\sin(\omega t_0)(1-e^{-\beta t}) + \frac{1}{\beta}\left[\int_0^t A(t')dt'-e^{-\beta t}\int_0^t A(t'')e^{\beta t''}dt''\right] . \tag{21}$$

Clearly $\langle x(t)\rangle_{\text{av}}=0$. Next we find

$$\langle x^2(t)\rangle_{\text{av}}=\frac{a^2}{2\beta^2}(1-e^{-\beta t})^2+\frac{1}{\beta^2}\sum_{i=1}^{3} I_i , \tag{22}$$

where

$$I_1=\int_0^t dt'\int_0^t \langle A(t')A(t'')\rangle_{\text{av}}dt''\simeq It , \tag{23}$$

$$I_2=-2\left[\int_0^t dt'\int_0^t dt''\,e^{\beta t''}\langle A(t')A(t'')\rangle_{\text{av}}\right]e^{-\beta t} \simeq -\frac{2I}{\beta}(1-e^{-\beta t}) , \tag{24}$$

and

$$I_3=e^{-2\beta t}\int_0^t dt'\,e^{\beta t'}\int_0^t dt''\,e^{\beta t''}\langle A(t')A(t'')\rangle_{\text{av}} \simeq \frac{I}{2\beta}(1-e^{-2\beta t}) . \tag{25}$$

In approximately evaluating the integrals I_1, I_2, and I_3, as before, on the coarser-time scale, we replaced t'' by t' and the limits in the integration with respect to t'' by $+\infty$. Thus, we get

$$\langle x^2(t)\rangle_{\text{av}}=\frac{1}{\beta^2}[\tfrac{1}{2}(a^2-3I/\beta)+(2I/\beta-a^2)e^{-\beta t} -\tfrac{1}{2}(a^2+I/\beta)e^{-2\beta t}+It] . \tag{26}$$

The asymptotic time behavior of $\langle x^2(t)\rangle_{\text{av}}$ is therefore

$$\langle x^2(t)\rangle_{\text{av}}=Dt+\frac{4}{m(pk\xi)^2}(\epsilon_0-\tfrac{3}{2}\xi) , \tag{27}$$

where the diffusion coefficient is given by

$$D=I/\beta^2=\frac{2}{mpk} . \tag{28}$$

Note, that when $t\to\infty$, $\langle V^2(t)\rangle_{\text{av}}$ and $\langle x^2(t)\rangle_{\text{av}}$ are independent of both the strength E_0 and frequency ω of the electromagnetic wave. Some other salient features of the obtained results are the smallness of

$$\langle W^2(\infty)\rangle_{\text{av}}=(\tfrac{1}{2}m\langle V^2(\infty)\rangle_{\text{av}}=\frac{\xi}{4}\ll\epsilon_0$$

and its independence on the collision frequency. Also, unexpectedly, D does not depend on ξ.

III. THE SIMULATION METHOD

In this section we describe a Monte Carlo computer experiment for testing predictions of the simplified theory presented in the preceding section. The main difficulty in the simulation of the diffusion process in our case is the rapid dependence of the electron energy and therefore also of the collision frequency on time. This complicates the simulation of time intervals elapsed between successive collisions. In order to overcome this difficulty, we adopt here the "null" event method;[6] namely, we introduce nonreal collisions characterized by collision frequency $\nu_{\text{null}}(\epsilon)$ such that the total collision frequency

$$\nu=\nu_{\text{null}}(\epsilon)+\nu_{\text{coll}}(\epsilon) \tag{29}$$

is energy independent. We are also assuming that the null

collisions do not perturb electron motion and, therefore, do not affect the results of the simulation.

The computer experiment proceeds as follows. We start with a test electron at a random-time moment t_0 at $x_0=0$, with zero initial velocity, and simulate the time interval τ_1 elapsed until the first collision takes place:[7]

$$\tau_1=-(\ln\psi_1)/\nu\ . \tag{30}$$

Here ψ_1 is a computer generated pseudorandom number with a uniform distribution in the interval (0,1). Next we use τ_1 to calculate the energy ϵ_1 of the electron just before the first collision takes place. Then we generate an additional pseudorandom number ψ_1' which serves to simulate the type of the collision. If $\nu_{\rm coll}(\epsilon_1)/\nu$ is less than ψ_1', we decide that a real inelastic collision takes place, otherwise the electron encounters a null collision. In the former case the electron velocity v_1^* and position x_1 just after the first collision is found from

$$\epsilon_1-\frac{mv_1^{*2}}{2}=\xi \tag{31}$$

and [see Eq. (4)]

$$x_1=x_0+V_0\tau_1+\frac{a}{\omega}[\cos(\omega t_1)-\cos(\omega t_0)]\ , \tag{32}$$

where $t_1=t_0+\tau_1$. In the case the first collision happens to be a null collision, x_1 is found in a similar way, and it is assumed that in the collision the velocity is unchanged ($\Delta_1=0$). At this point, we are ready to proceed to the simulation of the second collision. A new pseudorandom number ψ_2 is used to find the time interval $\tau_2=-(\ln\psi_2)/\nu$ between the first and the second collisions. The type of the second collision is then simulated so that we can find the new electron velocity increment Δ_2 and position x_2 immediately after the collision and so on. The simulation continues until the total elapsed time $\Delta t=\sum_i \tau_i$ exceeds a given value t. The actual position and velocity of the electron at t is then obtained. Finally, the whole simulation process is repeated with a sufficient number (usually $\sim 10^3$) of initial electrons at $x=0$, to provide the necessary statistics.

IV. RESULTS AND CONCLUSIONS

We applied the simulation scheme described in Sec. III for two gases N_2 and Hg. The corresponding total inelastic collision frequencies found from Refs. 8 and 9 (N_2) and Ref. 10 (Hg) are shown in Fig. 2 (solid lines). In the first simulation stage, we approximated the experimental graphs for $\nu_{\rm coll}(\epsilon)$ in Fig. 2 by the dashed curves, namely assumed that

$$\nu_{\rm coll}(\epsilon)=\begin{cases}0, & \epsilon<\xi\\ pk\epsilon, & \epsilon>\xi\end{cases} \tag{33}$$

where $\xi=11$ eV and $k=5.8\times10^7$ (sec eV Torr)$^{-1}$ for N_2, and $\xi=7.5$ eV and $k=3.4\times10^8$ (sec eV Torr)$^{-1}$ for Hg. Figure 3 shows the simulation results for $W=m/2\langle V^2\rangle_{\rm av}$ versus time in Hg for $\epsilon_0=30$ and 50 eV. Here and throughout the rest of the simulations, we used $\omega=30$ GHz and $p=1$ Torr. One can see in Fig. 3 the relaxation of the average electron energy W from its initial value of $\epsilon_0/2$ to a stationary value of ~ 1.9 eV which is in an excellent agreement with the predicted value of $\xi/4\simeq 1.87$ eV [see Eq. (19)]. Interesting to note, that even the initial relaxation phase of W agrees well with Eq. (22), as can be seen in Fig. 4, where we plot the results of the simulations for $W-\xi/4$ versus time. The slopes of these graphs yield, according to (22), the value of $\beta=1.5\times10^9$ (Torr sec)$^{-1}$, which is in a good agreement with the theoretical estimate [see Eq. (19)] of $\beta=1.27\times10^9$ (Torr sec)$^{-1}$.

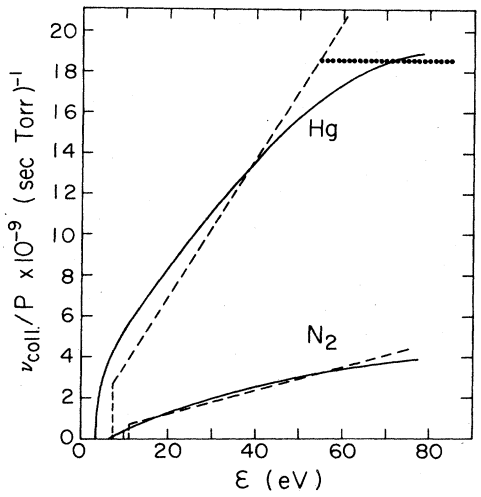

FIG. 2. Total inelastic electron-gas collision frequencies in N_2 and Hg (solid lines). The dashed lines represent a model with linear energy dependence used in the simulations. The dotted line for Hg ($\epsilon>55$ eV) represents an improved model for testing the limitations of the theory for large values of ϵ_0.

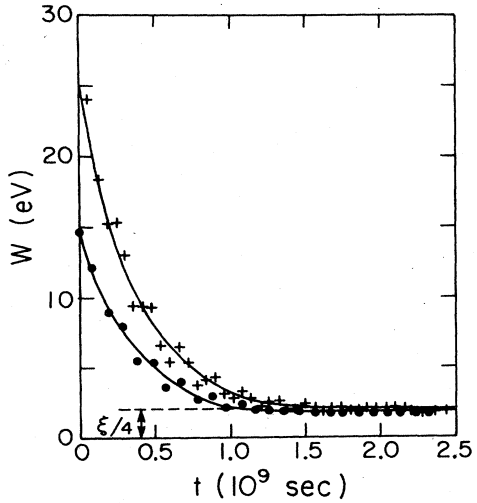

FIG. 3. Average translational energy $W=m/2\langle V^2\rangle_{\rm av}$ of the electrons in Hg versus time. ●, $\epsilon_0=30$ eV; , $\epsilon_0=50$ eV. The relaxation to the steady-state value $W=\xi/4$ is seen in the figure.

The results of the simulations for $\langle x^2\rangle_{av}$ versus time in N_2 and Hg are shown in Fig. 5. One can see that after a transition region and dependence $\langle x^2\rangle_{av}=Dt+B$ is established with $D=(3.7-5.1)\times10^7$ cm^{2}sec^{-1} Torr^{-1} in N_2 and $D=0.73\times10^7$ cm^{2}sec^{-1}Torr^{-1} in Hg. This agrees well with the theoretical predictions [Eq. (27)] of $D_{N_2}=6.1\times10^7$ cm^{2}sec^{-1}Torr^{-1} and $D_{Hg}=1.03\times10^7$ cm^{2}sec^{-1}Torr^{-1}. Note also that the values of B in Fig. 5 are much larger in the case on N_2, which also follows from Eq. (27) since $k_{N_2}\ll k_{Hg}$. This is why $\langle x^2\rangle_{av}$, for all times, in Hg is practically independent of ϵ_0. The weak dependence of D on ϵ_0 in N_2 is probably due to a poor satisfaction of the assumption of $\xi/\epsilon_0\ll1$ and to the vanishing of ν_{coll} for $\epsilon<\xi$, as used in the simulations.

In Fig. 6 we demonstrate the influence of the use in simulations of a more realistic collision frequency, for Hg at large electron energies (see the dotted line in Fig. 1)

$$\nu_{coll}(\epsilon)=\begin{cases}0, & \epsilon<\xi\\ pk\epsilon, & \xi<\epsilon<\epsilon_1\\ pk\epsilon_1, & \epsilon_1<\epsilon\ .\end{cases}\tag{34}$$

We can see in the figure that the improved collision model does not influence the previous results for D (the slope of the curves in the figure) significantly, as long as ϵ_0 is less than ϵ_1 (55 eV in our case). For $\epsilon_0>\epsilon_1$, the diffusion is faster, reflecting the reduction of the "effective" slope k of $\nu_{coll}(\epsilon)$ as compared to the simplified model (29).

In conclusion, we present the following summary.

(i) This work presents a theory of electron diffusion in a gas in the field of an intense electromagnetic wave for which the usual perturbative two-term expansion procedure in solving the Boltzmann equation is inapplicable.

(ii) Assuming $\omega\gg\nu_{coll}$, we had shown that the fast oscillations associated with the high-frequency electromagnetic wave can be averaged out, so that the diffusion process can be described on a slow (coarse) time scale by the Langevin type, model stochastic equation.

(iii) The shortness of the autocorrelation time $\tau=1/\langle\nu_{coll}\rangle_{av}$ in the Langevin equation in comparison to the relaxation time $1/\beta$, allows us to conveniently solve the model stochastic equation and to derive simple analytic expressions for the average electron translational energy W and the diffusion coefficient D.

(iv) In the case of a linear dependence of the inelastic collision frequency on electron energy, both W and D are shown to be independent of the strength and frequency of the electromagnetic wave.

(v) The theoretical predictions were found to be in a

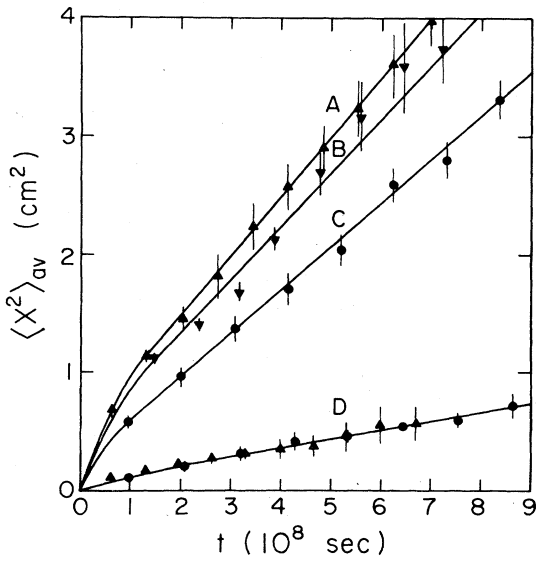

FIG. 5. Random-walk parameter $\langle x^2\rangle_{av}$ versus time in N_2 (curves A, B, and C) and Hg (curve D). ●, $\epsilon_0=30$ eV; ▼, $\epsilon_0=40$ eV; ▲, $\epsilon_0=50$ eV.

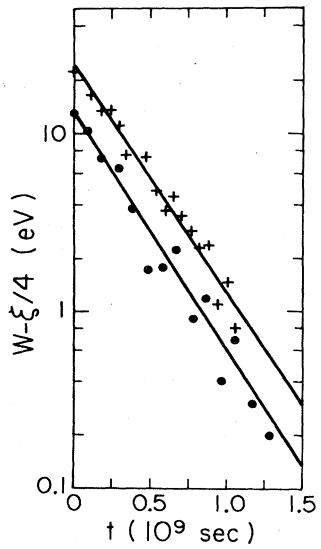

FIG. 4. Dependence of $W-\xi/4$ on time in Hg. ●, $\epsilon_0=30$ eV; +, $\epsilon_0=50$ eV. The slope of the curves in the figure is -2β.

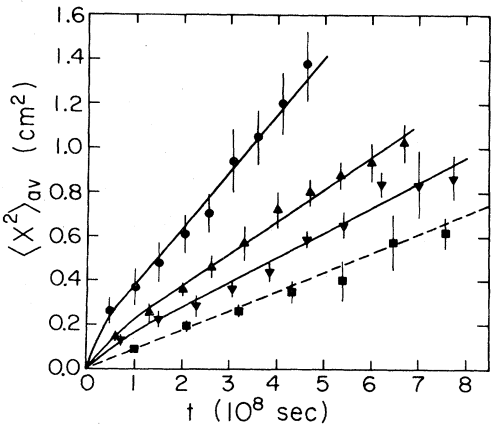

FIG. 6. Dependence of $\langle x^2\rangle_{av}$ on time for improved collision-frequency model in Hg. ■, $\epsilon_0=30$ eV; ▼, $\epsilon_0=40$ eV; ▲, $\epsilon_0=50$ eV; ●, $\epsilon_0=60$ eV. For comparison, the dashed line represents the simulation results obtained with a linear approximation for ν_{coll}.

good agreement with the results of the Monte Carlo computer experiments conducted for the cases of N_2 and Hg. The simulation scheme was considerably improved by using the null event method, and was also exploited in studying the deviations from the simplified theory, due to the violation of the aforementioned linear dependence of the collision frequency (usually at small or very large values of ϵ_0).

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