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Electronic Polarization of Atoms in Charged-Particle Impact

By

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Summary: The dependence of the polarization of an atom in charged-particle impact on the collision velocity is investigated by the impact-parameter method. An effective polarization potential for the elastic scattering is proposed. It has the form

$$V_p(r)=V_{ad.p}(r)\left(1+\frac{v^2}{\omega^2 r^2}\right)^{-1},$$

where $V_{ad.p}(r)$ is the usual adiabatic polarization potential, ω an adjustable parameter of the order of an effective excitation energy of the target divided by $\hbar$, and v the incident velocity.

It is confirmed that the induced dipole moment calculated by using the time-dependent perturbed atomic wave function and that given by the dynamic dipole polarizability are equivalent.

1. INTRODUCTION

The elastic collision of a charged particle with a neutral atom is discussed in this paper. When the incident energy is so low that the collision duration is longer than the period of orbital motion of atomic electrons, the effect of polarization of the target induced by the Coulomb field of the incident particle is expected to play an important role in determining a single-particle wave function $F(\boldsymbol{r}_0)$ of the scattered particle. The wave function $F(\boldsymbol{r}_0)$ may be defined by the projection of the wave function of the total system $\Psi(\boldsymbol{r}_0, \boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z)$ on the target wave function $\varphi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_Z\,;\,\boldsymbol{r}_0)$

$$F(\boldsymbol{r}_0)=\int \varphi^*(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_Z\,;\,\boldsymbol{r}_0)\Psi(\boldsymbol{r}_0, \boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z)d\boldsymbol{r}_1 d\boldsymbol{r}_2 \cdots d\boldsymbol{r}_Z,$$

where $\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_Z$ and $\boldsymbol{r}_0$ denote the position vectors of the atomic electrons and the incident particle, respectively. This definition has an ambiguity, because the target wave function $\varphi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_Z\,;\,\boldsymbol{r}_0)$ can be one of the unperturbed states or one of the perturbed states. Thus, the polarization potential is not uniquely defined. Nevertheless, in the energy region where inelastic processes are less important, it will be practically useful to consider such an approximate local potential as to be able to account for the observed angular distribution of elastically scattered particles.

In the low energy region, there have been many investigations [*1, 2*] on the polarization potential mostly based on the adiabatic approximation: the polariza-

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tion potential is calculated for each fixed distance between the target atom and the incident particle, by neglecting dynamic effects. During the past decade, however, there have been some investigations [*3–12*], which tried to take explicitly into account the nonadiabatic effects.

If the incident energy is very high, the first Born approximation without taking account of the polarization effect is expected to be applicable. In the intermediate energy region where the deviation from the first Born approximation becomes appreciable, the polarization potential should be taken into consideration [*13, 14*].

In most of the above-mentioned studies, the polarization potential does not explicitly depend on the incident velocity. It is clear that much more elaborate work than the usual adiabatic treatment is necessary to study the intermediate energy region where the polarization effect might depend on the collision velocity. It is a purpose of the present work to find out such an effective polarization potential. The potential may be used to predict an approximate differential cross section. Our discussions are restricted to distant collisions, in which the interaction between the target atom and the incident particle is mainly the polarization potential, and perturbation theory is expected to be a good approach to treat the problem. Several attempts are made within these limitations in §§ 2 and 3.

It is confirmed in § 4 that the induced dipole moment calculated by using time-dependent perturbed wave functions of the atom and that given by the dynamic dipole polarizability are equivalent. An effective polarization potential which depends on the incident velocity, and is primarily applicable to the small-angle scattering, is proposed in § 5.

2. Derivations of the Polarization Potential through a Reinterpretation of the Study of Massey and Mohr

As stated in the Introduction, our discussions are restricted to distant collisions. This means that the polarization potential may be the main part of interaction. Although the wave length of slow electrons is longer than an atomic radius, the semi-classical treatment may be permitted even in this case as long as distant collisions are considered. The concept of impact parameter may be introduced approximately when it is larger than the dimensions of the wave length of electrons. Furthermore, in such a distant collision, the incident wave of electrons may not be much distorted and thus the following discussions may be applicable approximately even to the electron scattering. The exchange between an atomic electron and the incident electron will be ignored. The atomic units will be used in the following equations.

It is assumed that the nucleus of the target atom has a charge Z and a sufficiently large mass and is fixed at the origin of our coordinate system. It is also assumed that an incident particle has a charge Z' and a mass m_0, and the target atom is neutral. The position vectors of the ith atomic electron and the incident particle are, respectively, denoted by $\boldsymbol{r}_i$ and $\boldsymbol{r}_0$. For brevity $\boldsymbol{r}$ and $\boldsymbol{r}_0^{-1}$ will be used to denote symbolically all the position vectors and those except $\boldsymbol{r}_0$, respectively. Spin coordi-

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nates of the incident particle need not be explicitly considered, because the effect of exchange is ignored and the spin-dependent term does not appear in our non-relativistic Hamiltonian. The reduced masses of the ith atomic electron and of the incident particle are denoted by μ_i and μ_0, respectively. The wave equation for the system of the atom and the incident particle is as follows

$$H(\boldsymbol{r})\Psi(\boldsymbol{r})=E\Psi(\boldsymbol{r}), \tag{1}$$

where H is the total Hamiltonian

$$H(\boldsymbol{r})=H_0(\boldsymbol{r}_0^{-1})-\frac{1}{2\mu_0}\nabla_0^2+V(\boldsymbol{r}), \tag{1-a}$$

$$H_0(\boldsymbol{r}_0^{-1})=\sum_{i=1}^{Z}\left(-\frac{1}{2\mu_i}\nabla_i^2-\frac{Z}{r_i}+\sum_{i>j=1}^{Z}\frac{1}{r_{ij}}\right), \tag{1-b}$$

$$V(\boldsymbol{r})=\frac{ZZ'}{r_0}-\sum_{i=1}^{Z}\frac{Z'}{r_{0i}}, \tag{1-c}$$

$$r_i=|\boldsymbol{r}_i|, \qquad r_{ij}=|\boldsymbol{r}_i-\boldsymbol{r}_j|, \tag{1-d}$$

and E is the total energy of the system. The eigenstates of atom are determined by the equation

$$H_0(\boldsymbol{r}_0^{-1})\Phi_n(\boldsymbol{r}_0^{-1})=E_n\Phi_n(\boldsymbol{r}_0^{-1}), \tag{2}$$

where the spin coordinates of atomic electrons should be explicitly considered. Here the function Φ_n and the quantity E_n are the eigenfunction and the eigenvalue of the nth state of the atom, respectively. The suffix n collectively represents a proper set of quantum numbers completely defining the state. Assuming that the eigenfunctions form a complete orthonormal set, we expand the total wave function $\Psi(\boldsymbol{r})$ into

$$\Psi(\boldsymbol{r})=\sum_{n=1}^{\infty}F_n(\boldsymbol{r}_0)\Phi_n(\boldsymbol{r}_0^{-1}). \tag{3}$$

The coefficients of the expansion $F_n(\boldsymbol{r}_0)$ should represent asymptotically an incident wave and scattered waves.

The first Born approximation becomes less satisfactory as the incident energy decreases from a high value to the energy region under consideration. This is because the distortion of the incident plane wave and the polarization of the target atom are not taken into account in this approximation. If we proceed to the second Born approximation, it is expected that these defects are somewhat removed. These effects are first considered by Massey and Mohr [*13*] forty years ago. They derived the following equation for the elastic scattering, to the second Born approximation,

$$[\nabla_0^2+k_1^2]F_1(\boldsymbol{r}_0)=U_{11}(\boldsymbol{r}_0)e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0}-\frac{1}{4\pi}\sum_{n=1}^{\infty}U_{1n}(\boldsymbol{r}_0)\int U_{n1}(\boldsymbol{r}')\frac{e^{ik_n|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}'. \tag{4}$$

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Here k_1 and k_n are the wave number of the incident particle and that of the scattered particle, respectively, and

$$k_n^2=2\mu_0(E-E_n), \tag{4-a}$$

$$U_{nm}(\boldsymbol{r}_0)=2\mu_0 V_{nm}(\boldsymbol{r}_0), \tag{4-b}$$

$$V_{nm}(\boldsymbol{r}_0)=\int \Phi_n^*(\boldsymbol{r}_0^{-1})V(\boldsymbol{r})\Phi_m(\boldsymbol{r}_0^{-1})d\boldsymbol{r}_0^{-1}, \tag{4-c}$$

and $\boldsymbol{n}_0$ is a unit vector in the incident direction which we take in the direction of the z-axis. Using the fact that the wave function $\Phi_n(\boldsymbol{r}_0^{-1})$ may be chosen to be real, the matrix elements $V_{nm}(\boldsymbol{r}_0)$ are always real. If the right hand side of Eq. (4) is approximated by $U_{eff}(\boldsymbol{r}_0)F_1(\boldsymbol{r}_0)$, the quantity $U_{eff}(\boldsymbol{r}_0)/(2\mu_0)$ may be called the effective potential in the elastic scattering. The scattered particle feels it as an average field. Therefore Eq. (4) is rewritten as follows

$$[\nabla_0^2+k_1^2]F_1(\boldsymbol{r}_0)=U_{eff}(\boldsymbol{r}_0)F_1(\boldsymbol{r}_0). \tag{5}$$

By replacing $F_1(\boldsymbol{r}_0)$ on the right hand side of Eq. (5) by the plane wave $\exp(ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0)$ and comparing with the right hand side of Eq. (4), the explicit form of $U_{eff}(\boldsymbol{r}_0)$ is determined. The correction terms to the static potential $U_{11}(\boldsymbol{r}_0)/(2\mu_0)$ in $U_{eff}(\boldsymbol{r}_0)/(2\mu_0)$ approximately contain the effect of the distortion of the incident plane wave, represented by the term $n=1$, and that of the polarization of the target atom, arising from the others. As given by Massey and Mohr, the polarization potential $V_p(\boldsymbol{r}_0)$ is thus obtained as follows

$$V_p(\boldsymbol{r}_0)=-\frac{2\mu_0}{4\pi}e^{-ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0}\sum_{n\neq 1}^{\infty}V_{1n}(\boldsymbol{r}_0)\int V_{n1}(\boldsymbol{r}')\frac{e^{ik_n|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}'. \tag{6}$$

The approximations used above would be fairly good, when the effective potential obtained is small as compared with the incident energy. The polarization potential derived here is a complex potential. It seems that such a potential contains some elements other than the polarization potential in the elastic scattering. We discuss this inference in the following.

The total cross section for an excitation obtained by making use of the nth Born approximation is known to be practically equal to that obtained by the impact parameter method when the collision energy is sufficiently high [*15, 16*]. It is expected, therefore, that a formula equivalent to Eq. (6) may be derived by using the impact parameter method. This is done in § 3.1. We here rewrite Eq. (6) into a form which can be directly compared with the result of calculations in § 3.1. It is convenient to write (see Fig. 1)

$$\boldsymbol{r}_0=\boldsymbol{b}+\boldsymbol{n}_0 z,\ z=vt, \quad \text{and} \quad \boldsymbol{b}\cdot\boldsymbol{n}_0=0, \tag{7}$$

where the incident particle is assumed to move along a straight line running parallel to the z-axis, the origin of time t is taken at the point of closest approach, and the velocity of the incident particle v and the impact parameter b are assumed constant

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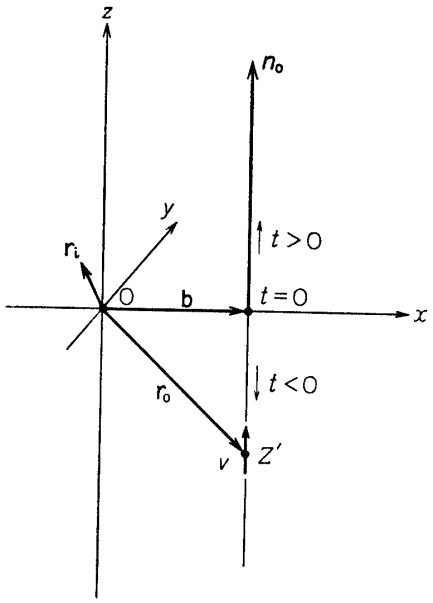

FIG. 1. Coordinates for the collision of a charged-particle and an atom.

throughout the collision process. In the same way as done by Moiseiwitsch [*16*], we assume that the approximation,

$$k_1 \cong k_n \cong \mu_0 v \quad \text{and} \quad (k_1\boldsymbol{n}_0 - k_n\boldsymbol{n})\cdot\boldsymbol{n}_0 \cong \frac{1}{2k_1}(k_1^2-k_n^2) \cong \frac{\omega_{n1}}{v}, \qquad (8)$$

are permitted. Making the Fourier transformation of the factor $\exp(ik_n|\boldsymbol{r}_0-\boldsymbol{r}'|)/|\boldsymbol{r}_0-\boldsymbol{r}'|$ in the integrand in Eq. (6), substituting Eq. (7) into the transformed expression of Eq. (6), and making use of the well-known relations of δ-function and step-function, we obtain the complex polarization potential

$$V_p(t) = -i\sum_{n\neq 1}^{\infty}\int_{-\infty}^{t} dt_1 V_{1n}(t)V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}. \qquad (9)$$

The real part and the imaginary one are more easily separated from the complex polarization potential in Eq. (9) than in Eq. (6). In general, as Mott and Massey [*17*] have shown by the wave mechanical method, the negative imaginary part of a potential in a scattering equation means that the equation takes an explicit account of the occurrence of an inelastic scattering. This will be shown, if the time variation of the probability amplitude is considered by the impact parameter method.

As usual, we start from the following time-dependent equation

$$i\frac{\partial}{\partial t}\psi(\boldsymbol{r}_0^{-1}, t) = \mathscr{H}(\boldsymbol{r}_0^{-1}, t)\psi(\boldsymbol{r}_0^{-1}, t). \qquad (10)$$

It has been shown by several authors [*18*] that the equation (10) is approximately equivalent to the equation (1). By the transformation of Eq. (7), $V(\boldsymbol{r})$ and $H(\boldsymbol{r})$

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in Eq. (1) are now regarded as $V(\boldsymbol{r}_0^{-1}, t)$ and $\mathscr{H}(\boldsymbol{r}_0^{-1}, t)$, respectively. The function $\phi(\boldsymbol{r}_0^{-1}, t)$ is a time-dependent wave function of the atom. It is expanded in terms of the unperturbed atomic wave functions $\Phi_n(\boldsymbol{r}_0^{-1})$ into

$$\phi(\boldsymbol{r}_0^{-1}, t)=\sum_{n=1}^{\infty} C_n(t)\Phi_n(\boldsymbol{r}_0^{-1})e^{-iE_nt}. \tag{11}$$

Here, as is well-known, $C_n(t)$ is determined by

$$i\frac{d}{dt}C_n(t)=\sum_{m=1}^{\infty} V_{nm}(t)C_m(t)e^{i\omega_{nm}t}, \tag{12}$$

where

$$\omega_{nm}=E_n-E_m. \tag{12-a}$$

The solution of Eq. (12), to the first approximation, is given by

$$C_n^{(1)}(t)=\delta_{n1}-i\int_{-\infty}^{t} dt_1 V_{n1}(t_1)e^{i\omega_{n1}t_1}. \tag{13}$$

The diagonal term $V_{nn}(t)$ on the right hand side of Eq. (12) contributes to the elastic cross section, while the nondiagonal terms $V_{nm}(t)$ are mainly effective in those of the inelastic scattering. Instead of solving Eq. (12), we take into account the effect of inelastic scattering on the elastic scattering by adding the matrix element of a negative imaginary potential $\{-i\mathscr{V}(t)\}$ for the nth state of target atom to the diagonal term $V_{nn}(t)$. From Eq. (12) the probability amplitude of the ground state channel satisfies the following equation

$$i\frac{d}{dt}C_1(t)=(V_{11}-i\mathscr{V}_{11})C_1(t), \tag{14}$$

where $\mathscr{V}_{11}(t)$ is the matrix element of the $\mathscr{V}(t)$ for the ground state target. The solution of Eq. (14) with the initial condition $C_1(-\infty)=1$ is given by

$$C_1(t)=\exp\left\{-\int_{-\infty}^{t} dt_1\mathscr{V}_{11}(t_1)-i\int_{-\infty}^{t} dt_1 V_{11}(t_1)\right\}. \tag{15}$$

In this approximation,

$$|C_1(t)|^2\cong 1-2\int_{-\infty}^{t} dt_1\mathscr{V}_{11}(t_1). \tag{16}$$

To determine the form of $\mathscr{V}_{11}(t)$, we make use of the conservation of probability

$$|C_1(t)|^2=1-\sum_{n\neq 1}^{\infty}|C_n(t)|^2. \tag{17}$$

Comparing Eq. (16) with Eq. (17), and substituting $C_n(t)$ from Eq. (13), we obtain

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$$-i\mathscr{V}_{11}(t)=-i\sum_{n\neq 1}^{\infty}\int_{-\infty}^{t}dt_1 V_{1n}(t)V_{n1}(t_1)\cos\omega_{n1}(t-t_1).$$

This is exactly the imaginary part of the complex polarization potential $V_p(t)$ in Eq. (9). As seen from Eq. (16), the existence of this potential reduces the probability that the target atom is in the ground state. Thus the imaginary potential should be excluded from the effective polarization potential for the elastic scattering. Furthermore, when the real excitations occur, the energy of the atom gained through the excitation contributes to the real part of $V_p(t)$ in Eq. (9). It is not known how this contribution of the excitation can be removed in an unambiguous manner. This may limit the validity of the concept of the effective polarization potential.

In the low energy region, where the real excitation does not take place, it is shown that Eq. (6) reduces to the usual adiabatic polarization potential in the limit of the infinitely slow motion of the incident particle relative to the target atom. Even in such a low-energy collision, the distortion of the plane wave is not so remarkable as long as distant collisions are considered. We can obtain the scattering equations by the well-known procedures

$$[\nabla_0^2+k_1^2]F_1(\boldsymbol{r}_0)=\sum_{n=1}^{\infty}U_{1n}(\boldsymbol{r}_0)F_n(\boldsymbol{r}_0), \tag{18-a}$$

$$[\nabla_0^2-\kappa_n^2]F_n(\boldsymbol{r}_0)=\sum_{m=1}^{\infty}U_{nm}(\boldsymbol{r}_0)F_m(\boldsymbol{r}_0), \tag{18-b}$$

where

$$E=\frac{1}{2\mu_0}k_1^2+E_1=-\frac{1}{2\mu_0}\kappa_n^2+E_n, \qquad \text{for } n\neq 1. \tag{18-c}$$

We are able to conclude, to the second order approximation, that the form of the complex polarization potential $V_p(\boldsymbol{r}_0)$ in Eq. (6) remains valid, but the wave number k_n should be replaced by $-i\kappa_n$ for $n\neq 1$.

$$V_p(\boldsymbol{r}_0)=-\frac{2\mu_0}{4\pi}e^{-ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0}\sum_{n\neq 1}^{\infty}V_{1n}(\boldsymbol{r}_0)\int V_{n1}(\boldsymbol{r}')\frac{e^{-\kappa_n|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}'. \tag{19}$$

As we have assumed $r_0\gg 1$, the order of magnitude of $V_{n1}(\boldsymbol{r})$ is

$$V_{n1}(\boldsymbol{r})\sim\frac{1}{r^2}. \tag{19-a}$$

This is the behavior of the dipole interaction for the allowed transition between the nth state and the ground state. As, in the integrand of Eq. (19), the matrix element $V_{n1}(\boldsymbol{r})$ is a slowly varying function of $\boldsymbol{r}$ and the factor $\exp(-\kappa_n|\boldsymbol{r}_0-\boldsymbol{r}|)/|\boldsymbol{r}_0-\boldsymbol{r}|$ contributes to the integral mainly in the vicinity of $\boldsymbol{r}_0$, it will be permitted to approximate the latter as follows

$$\frac{e^{-\kappa_n|\boldsymbol{r}_0-\boldsymbol{r}|}}{|\boldsymbol{r}_0-\boldsymbol{r}|}\sim\frac{4\pi}{\kappa_n^2}\delta(\boldsymbol{r}_0-\boldsymbol{r}), \tag{20}$$

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with the normalization factor. For an incident energy which is negligibly small as compared with the lowest excitation energy, Eq. (19) reduces to the usual adiabatic expression

$$V_{ad.p}(\boldsymbol{r}_0) \sim -\sum_{n\neq 1}^{\infty} \frac{|V_{n1}(\boldsymbol{r}_0)|^2}{E_n - E_1}, \tag{21}$$

where the approximation Eq. (20) has been used. Because κ_2 is nearly zero for the incident energy near the threshold of the first excitation energy, the approximation Eq. (20) is not permitted in such a case. The adiabatic approximation may get less satisfactory for such incident energy region. Further discussions are given concerning the validity of the adiabatic potential in § 5.

As stated under Eq. (17), the complex polarization potential defined by Eq. (6) generally contains the effect of excitations. It is anticipated that such effect may be separated into several terms, say the excitation energy and the permanent multipole interaction, in the asymptotic form. We investigate the asymptotic form in the following. The asymptotic form for a moderately low incident energy is derived in the limit of $t \to -\infty$ from the real part of Eq. (9) by integrating by parts and by using the condition $V_{1n}(\pm\infty) \cong 0$ as follows

$$V_p(r_0) \sim -\frac{\alpha Z'^2}{2r_0^4} + \frac{6v^2 Z'^2}{2r_0^6} \sum_{n\neq 1}^{\infty} \frac{\alpha_n}{\omega_{n1}^2} + O\left(\frac{1}{r_0^7}\right), \tag{22}$$

where

$$\alpha = \sum_{n\neq 1}^{\infty} \alpha_n = \sum_{n\neq 1}^{\infty} \frac{2\left\langle 1 \left| \sum_{i=1}^{Z} (-\boldsymbol{r}_i) \right| n \right\rangle \left\langle n \left| \sum_{i=1}^{Z} (-\boldsymbol{r}_i) \right| 1 \right\rangle}{\omega_{n1}}, \tag{22-a}$$

is the dipole polarizability of the atom. In the limit of $t \to +\infty$, the permanent dipole potential and so forth are added to Eq. (22). The term due to the dipole interaction has the form

$$\frac{Z'\boldsymbol{P}\cdot\boldsymbol{r}_0}{2r_0^3} \cong \frac{Z'b}{2r_0^3} P_x + \frac{Z'}{2r_0^3} P_z \left(r_0 - \frac{b^2}{2r_0}\right). \tag{22-b}$$

When a hydrogen atom is considered as the target, the asymptotic forms of the x- and z-components of dipole moment are given respectively by

$$P_x \underset{t\to+\infty}{\sim} -\sum_{n\neq 1}^{\infty} \frac{2Z'}{v^2} \alpha_n \omega_{n1}^2 K_1\left(\frac{b\omega_{n1}}{v}\right) \sin \omega_{n1} t, \tag{22-c}$$

$$P_z \underset{t\to+\infty}{\sim} \sum_{n\neq 1}^{\infty} \frac{2Z'}{v^2} \alpha_n \omega_{n1}^2 K_0\left(\frac{b\omega_{n1}}{v}\right) \cos \omega_{n1} t, \tag{22-d}$$

where K_0 and K_1 are the modified Bessel functions of the second kind. The second term in Eq. (22) well represents the physical situation. As the incident velocity v becomes large within the restriction $(v/\omega_{n1}) < r_0$, the target atom is less polarized.

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Thus the polarization potential becomes smaller, as the velocity of incident particle increases. For a high incident energy, where the approximation $k_n \cong k_1$ is permitted, when we consider a hydrogen atom as the target, the asymptotic form of Eq. (6) is represented by

$$V_p(r_0) \sim -\frac{2(1-3\cos\theta)}{k_1^2 r_0^4}\left\{1-\frac{\cos 2k_1 r_0}{(1+4k_1^2)^3}\right\}+O\left(\frac{1}{r_0^5}\right). \tag{23}$$

This is obtained by excluding the imaginary parts from the asymptotic expression which Massey and Mohr have already shown. The main term of Eq. (23) is positive for the scattering angle θ which satisfies $\cos\theta > 1/3$. This expression is valid when $k_n \cong k_1$. This peculiar behavior which is quite contrary to the usual adiabatic polarization potential may be due to the nonadiabatic effect.

3. Other Derivations of the Polarization Potential

3.1. *The Second Order Approximation in the Impact Parameter Method*

Let's directly derive Eq. (9), which, in the last section, is given by the reduction of the wave mechanical equation (6), by making use of the impact parameter treatment. The solution of Eq. (12) for the elastic scattering is obtained, to the second order approximation, as

$$\begin{aligned} C_1^{(2)}(t) &= 1+(-i)\int_{-\infty}^{t} dt_1\left[V_{11}(t_1)+(-i)\sum_{n=1}^{\infty} V_{1n}(t_1)\int_{-\infty}^{t_1} dt_2 V_{n1}(t_2)e^{-i\omega_{n1}(t_1-t_2)}\right] \\ &\equiv 1+(-i)\int_{-\infty}^{t} dt_1 V_{eff}(t_1), \end{aligned} \tag{24}$$

where V_{eff} is the effective potential corresponding to $U_{eff}(r_0)/(2\mu_0)$ in § 2. As noted under Eq. (5), the correction terms to the static potential $V_{11}(t)$ in $V_{eff}(t)$ represent the effect of distortion of the orbital motion of the incident particle by the target atom and that of polarization of the target atom. The complex polarization potential is given by

$$V_p(t) = -i\sum_{n\neq 1}^{\infty}\int_{-\infty}^{t} dt_1 V_{1n}(t)V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}. \tag{25}$$

This expression is exactly the same as Eq. (9). This equality is a particular case of the Moiseiwitsch's conclusion.

For the incident energy lower than any excitation energy of atoms, we are able to show that Eq. (25) is also reduced to the usual adiabatic polarization potential. Integrating Eq. (25) by parts, we obtain

$$V_p(t) = -\sum_{n\neq 1}^{\infty}\frac{|V_{n1}(t)|^2}{\omega_{n1}}+\sum_{n\neq 1}^{\infty}\frac{V_{1n}(t)}{\omega_{n1}}e^{-i\omega_{n1}t}\int_{-\infty}^{t} dt_1\frac{\partial V_{n1}(t_1)}{\partial t_1}e^{i\omega_{n1}t_1}. \tag{25-a}$$

We transform the integration variable t into z according to Eq. (7). As the factors

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$\partial V_{n1}(v/z)/\partial z$ and $\exp(i\omega_{n1}z/v)$ in the integrand are, respectively, a slowly varying function and very rapidly varying function of z, the contribution of the second integral term to the $V_p(t)$ in Eq. (25–a) is negligibly small as compared with that of the first term. Equation (25) is thus reduced to the usual adiabatic polarization potential

$$V_p(\boldsymbol{r}_0) \cong -\sum_{n\neq 1}^{\infty} \frac{|V_{n1}(\boldsymbol{r}_0)|^2}{E_n - E_1}, \tag{25–b}$$

where the variable is transformed by making use of Eq. (7).

As the imaginary term should be excluded in Eq. (25), the polarization potential is given by

$$V_p(t) = -\sum_{n\neq 1}^{\infty} \int_{-\infty}^{t} dt_1 V_{1n}(t) V_{n1}(t_1) \sin \omega_{n1}(t-t_1). \tag{26}$$

When excitations occur, the asymptotic form of Eq. (26) in the limit $t \to +\infty$ includes the dipole potential and so forth as mentioned before. Thus the effective polarization potential for the elastic scattering is not unambiguously defined throughout the scattering processes.

3.2. *The Expectation Value of Energy of the System*

The change in the internal energy of target atom (denoted by V_{in}) induced by the interaction with the incident particle is regarded as a sum of the energy due to the polarization of the atom and the excitation energy gained through a real electronic excitation. It is defined by

$$V_{in}(\boldsymbol{r}_0) = \langle \psi(\boldsymbol{r}_0^{-1}, \boldsymbol{r}_0) | H | \psi(\boldsymbol{r}_0^{-1}, \boldsymbol{r}_0) \rangle - \langle \Phi_1(\boldsymbol{r}_0^{-1}) | H | \Phi_1(\boldsymbol{r}_0^{-1}) \rangle, \tag{27}$$

where $\psi(\boldsymbol{r}_0^{-1}, \boldsymbol{r}_0)$ is the wave function of the atom perturbed by the incident particle. The effective polarization potential for the elastic scattering is the internal energy temporarily increased of target atom under scattering processes. If the incident energy is lower than the lowest excitation energy of atoms, an effective polarization potential is given by the definition Eq. (27). When the incident energy is so high that electronic excitations occur, an effective polarization potential may be obtained by the subtraction of the excitation energy from Eq. (27). As the expected value of the excitation energy is constant in the asymptotic region, it is possible to subtract its value from the asymptotic form of Eq. (27) to obtain the polarization potential. In the short and intermediate distances from the origin, the distinction between temporary excitations and real excitations is not possible. We restrict our discussions to distant collisions. We may therefore use the perturbation method in the impact parameter treatment. The wave function $\psi(\boldsymbol{r}_0^{-1}, \boldsymbol{r}_0)$ and Hamiltonian H in Eq. (27) are approximated by $\psi(\boldsymbol{r}_0^{-1}, t)$ and $\mathscr{H}(\boldsymbol{r}_0^{-1}, t)$ as introduced in § 2, respectively. Equation (27) is represented, to the second order with respect to the interaction potential $V(\boldsymbol{r}_0^{-1}, t)$, by

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$$V_{in}(t)=\sum_{n\neq 1}^{\infty}\omega_{n1}|C_n^{(1)}(t)|^2 + \sum_{n\neq 1}^{\infty}\left[(-i)\frac{dC_n^{(1)*}(t)}{dt}C_n^{(1)}(t)+\left\{(-i)\frac{dC_n^{(1)*}(t)}{dt}C_n^{(1)}(t)\right\}^*\right]$$
$$\cong\sum_{n\neq 1}^{\infty}\omega_{n1}\left|-i\int_{-\infty}^{t}dt_1V_{n1}(t_1)e^{i\omega_{n1}t_1}\right|^2 + 2\,\mathrm{Re}\left[\sum_{n\neq 1}^{\infty}(-i)\int_{-\infty}^{t}dt_1V_{1n}(t)V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}\right]+O(V^3). \quad (28)$$

The first term on the right hand side of Eq. (28) is the expectation value of the excitation energy.

When real excitations occur, we have to investigate whether the effect of excitation can be separated from $V_{in}(\boldsymbol{r}_0)$ or not. We shall start from the wave mechanical treatment. We first consider the incident energy that is higher than any excitation energy of atoms. Which terms then should be removed from $V_{in}(\boldsymbol{r}_0)$ to obtain the effective polarization potential? We try to answer this question as follows.

If the distortion of the incident plane wave and the polarization of the target atom are unable to neglect, as mentioned by Massey and Mohr, we need to proceed at least to the second Born approximation:

$$[\nabla_0^2+k_1^2]F_1(\boldsymbol{r}_0)=U_{11}(\boldsymbol{r}_0)e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0} - \frac{1}{4\pi}\sum_{n=1}^{\infty}U_{1n}(\boldsymbol{r}_0)\int U_{n1}(\boldsymbol{r}')\frac{e^{ik_n|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}', \quad (29)$$

$$[\nabla_0^2+k_n^2]F_n(\boldsymbol{r}_0)=U_{n1}(\boldsymbol{r}_0)e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0} - \frac{1}{4\pi}\sum_{m=1}^{\infty}U_{nm}(\boldsymbol{r}_0)\int U_{m1}(\boldsymbol{r}')\frac{e^{ik_m|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}', \quad (30)$$

A state of scattered particle under collision processes is described by the wave function of relative motion $F_1(\boldsymbol{r}_0)$ or $F_n(\boldsymbol{r}_0)$. Although the incident particle is scattered by the target, the direction of scattered particle would not be much deflected from the incident direction and the scattered wave functions would be represented by the plane waves with a slowly varying amplitude as long as the high incident energy is assumed. Thus we put

$$F_1(\boldsymbol{r}_0)=C_1(\boldsymbol{r}_0)e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0} \quad \text{and} \quad F_n(\boldsymbol{r}_0)=C_n(\boldsymbol{r}_0)e^{ik_n\boldsymbol{n}\cdot\boldsymbol{r}_0},$$

in the right hand side of Eqs. (29) and (30), respectively, and rewrite them as follows

$$[\nabla_0^2+k_1^2]F_1(\boldsymbol{r}_0)=2\mu_0\left[\frac{V_{11}(\boldsymbol{r}_0)}{C_1(\boldsymbol{r}_0)}-\frac{e^{-ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0}}{C_1(\boldsymbol{r}_0)}\frac{2\mu_0}{4\pi} \times\sum_{n=1}^{\infty}\int V_{1n}(\boldsymbol{r}_0)V_{n1}(\boldsymbol{r}')\frac{e^{ik_n|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}'\right]F_1(\boldsymbol{r}_0), \quad (29\text{-a})$$

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$$[\nabla_0^2+k_1^2]F_n(\boldsymbol{r}_0)=2\mu_0\Big[\omega_{n1}+\frac{e^{-ik_n\boldsymbol{n}\cdot\boldsymbol{r}_0}}{C_n(\boldsymbol{r}_0)}\Big\{V_{n1}(\boldsymbol{r}_0)\,e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0}-\frac{2\mu_0}{4\pi}\times\sum_{m=1}^{\infty}\int V_{nm}(\boldsymbol{r}_0)V_{m1}(\boldsymbol{r}')\frac{e^{ik_m|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}'\Big\}\Big]F_n(\boldsymbol{r}_0). \tag{30–a}$$

We assume $C_n(\boldsymbol{r}_0)$ as a slowly varying function of $\boldsymbol{r}_0$. There is no guarantee for the relation $\sum_{n=1}^{\infty}|C_n(\boldsymbol{r}_0)|^2=1$. We are able to regard the function $C_n(\boldsymbol{r}_0)$ as the amplitude corresponding to the excitation of the atom to the nth state. These amplitudes may be approximated by $C_n^{(1)}(t)$ given in Eq. (13). This is because the wave function $F_n(\boldsymbol{r}_0)$ is the coefficient of eigenfunction expansion of the total wave function as in Eq. (3). It is expected from the above discussions and Eqs. (29–a) and (30–a) that the effective interaction acting on the scattered wave will be given as follows

$$\begin{aligned}&|C_1(\boldsymbol{r}_0)|^2\Big\{\frac{V_{11}(\boldsymbol{r}_0)}{C_1(\boldsymbol{r}_0)}-\frac{e^{-ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0}}{C_1(\boldsymbol{r}_0)}\frac{2\mu_0}{4\pi}\sum_{n=1}^{\infty}\int V_{1n}(\boldsymbol{r}_0)V_{n1}(\boldsymbol{r}')\frac{e^{ik_n|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}'\Big\}\\&+\sum_{n\neq1}^{\infty}|C_n(\boldsymbol{r}_0)|^2\Big[\omega_{n1}+\frac{e^{-ik_n\boldsymbol{n}\cdot\boldsymbol{r}_0}}{C_n(\boldsymbol{r}_0)}\Big\{V_{n1}(\boldsymbol{r}_0)\,e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}_0}-\frac{2\mu_0}{4\pi}\\&\times\sum_{m=1}^{\infty}\int V_{nm}(\boldsymbol{r}_0)\,V_{m1}(\boldsymbol{r}')\frac{e^{ik_m|\boldsymbol{r}_0-\boldsymbol{r}'|}}{|\boldsymbol{r}_0-\boldsymbol{r}'|}e^{ik_1\boldsymbol{n}_0\cdot\boldsymbol{r}'}d\boldsymbol{r}'\Big\}\Big].\end{aligned}$$

The terms due to the polarization of atom in the above expression are given by

$$\begin{aligned}&|C_1^{(1)}(t)|^2\Big\{-\frac{i}{C_1^{(1)}(t)}\sum_{n\neq1}^{\infty}\int_{-\infty}^{t}dt_1V_{1n}(t)V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}\Big\}\\&+\sum_{n\neq1}^{\infty}|C_n^{(1)}(t)|^2\Big[\omega_{n1}+\frac{1}{C_n^{(1)}(t)}\Big\{V_{n1}(t)e^{i\omega_{n1}t}\\&-i\sum_{m=1}^{\infty}\int_{-\infty}^{t}dt_1V_{nm}(t)V_{m1}(t_1)e^{-i\omega_{m1}(t-t_1)}\Big\}\Big]\\&\cong\sum_{n\neq1}^{\infty}(-i)\int_{-\infty}^{t}dt_1V_{1n}(t)V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}+\sum_{n\neq1}^{\infty}\omega_{n1}\Big|-i\int_{-\infty}^{t}dt_1V_{n1}(t_1)e^{i\omega_{n1}t_1}\Big|^2\\&+\Big\{\sum_{n\neq1}^{\infty}(-i)\int_{-\infty}^{t}dt_1V_{1n}(t)V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}\Big\}^*+O(V^3),\end{aligned} \tag{31}$$

where $C_n(\boldsymbol{r}_0)$ is approximated by $C_n^{(1)}(t)$ in Eq. (13), the transformation Eq. (7) and the approximation Eq. (8) are used, and the same procedures that are made to transform Eq. (6) into Eq. (9) are used. This expression Eq. (31) is exactly identical with Eq. (28). The first term on the right hand side of Eq. (31) originates from the elastic scattering equation (29-a), and the second and third terms from the inelastic scattering equation (30-a). It seems that the question at the beginning of the last paragraph is answered. But these discussions are by no means sufficient. As the first term on the right hand side of Eq. (31) that is the same form as Eq. (9) contains the imaginary part, such term involves the effect of the inelastic scattering as discussed in § 2. The question how any excitation energy is removed from Eqs. (27) or (28) for the elastic scattering still remains to be answered in the short

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and intermediate regions. The effective polarization potential based on the asymptotic form is discussed in § 5.

For the incident energy lower than the lowest excitation energy of atoms, we are able to show that $V_{in}(t)$ is reduced to the adiabatic polarization potential, if we apply the same procedures that are used to transform Eq. (25) into Eq. (25-b).

For an intermediate incident energy, we may define the polarization potential by V_{in} in Eqs. (27) or (28) as long as distant collisions are considered, because the effect of excitations is negligibly small. That this is permitted is seen from the discussion about the adiabatic limit and also from Figs. 2 and 3. The discussions about Figs. 2 and 3 are given in § 3. 4. The asymptotic form of $V_{in}(t)$ in Eq. (28) is derived in the limit of $t\to-\infty$ by using the integration by parts

$$V_p(r_0)\sim-\frac{\alpha Z'^2}{2r_0^4}+\frac{4v^2Z'^2}{2r_0^6}\sum_{n\neq1}^{\infty}\frac{\alpha_n}{\omega_{n1}^2}+O\left(\frac{1}{r_0^7}\right), \tag{32}$$

where $\alpha=\sum_{n\neq1}^{\infty}\alpha_n$ is the dipole polarizability of the atom defined by Eq. (22-a). If we replace $1/\omega_{n1}^2$ by an average value $1/\omega^2$ and take it out of the summation in the second term of Eq. (32), Eq. (32) is written as

$$V_p(r_0)\sim-\frac{\alpha Z'^2}{2r_0^4}\left(1-\frac{4v^2}{\omega^2r_0^2}\right)+O\left(\frac{1}{r_0^7}\right). \tag{32-a}$$

In the limit of $t\to+\infty$, the excitation energy, the permanent dipole interaction, and so forth are added to Eq. (32). But the difference in the definition of the polarization potential brings the numerical factor 4 in the second term of Eq. (32) instead 6 in that of Eq. (22).

3.3. *The Work Done by the Induced-Dipole Interaction on the Incident Particle*

The polarization of the atom due to the Coulomb field of the incident particle is mainly reflcted by the induced dipole moment $\boldsymbol{P}$, provided the induced quadrupole and higher multipole moments are negligibly small as compared with the induced dipole moment. The potential field produced at a point $\boldsymbol{r}_0$ by a point dipole $\boldsymbol{P}$ at the origin of the coordinate system is given by

$$V(\boldsymbol{r}_0)=\frac{\boldsymbol{P}\cdot\boldsymbol{r}_0}{r_0^3}. \tag{33}$$

The strength of the electric field at $\boldsymbol{r}_0$ is

$$\boldsymbol{F}(\boldsymbol{r}_0)=-\text{grad}\,V(\boldsymbol{r}_0), \tag{34}$$

where $\boldsymbol{P}(\boldsymbol{r}_0)$ is regarded as constant in performing the 'grad' operation.

To move a particle with charge Z' from $r_0=-\infty$ to any point $\boldsymbol{r}_0$ along a straigh line running parallel to the z-axis against the electric field $\boldsymbol{F}(\boldsymbol{r}_0)$ (see Fig. 1 for the coordinate system), a work

$$W(\boldsymbol{r}_0)=-Z'\int_{-\infty}^{z}\boldsymbol{F}(z_1)\cdot\boldsymbol{k}dz_1=Z'\int_{-\infty}^{z}\frac{\partial}{\partial z_1}\left\{\frac{\boldsymbol{P}(z_1)\cdot\boldsymbol{r}_1}{r_1^3}\right\}dz_1, \tag{35}$$

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is needed. Here $\boldsymbol{k}$ is a unit vector in the direction of z-axis. In differentiating $\{\boldsymbol{P}(z)\cdot\boldsymbol{r}/r^3\}$ with respect to z in the integrand of Eq. (35), $\boldsymbol{P}(z)$ is regarded as constant. After the differentiation, the dependence of $\boldsymbol{P}(z)$ on z must be retained. Equation (35) is thus reduced to

$$W(\boldsymbol{r}_0)=\frac{Z'\boldsymbol{P}(z)\cdot\boldsymbol{r}_0}{r_0^3}-Z'\int_{-\infty}^{z}\frac{1}{r_1^3}\left\{\boldsymbol{r}_1\cdot\frac{d\boldsymbol{P}(z_1)}{dz_1}\right\}dz_1. \tag{36}$$

It is shown below that this work is equal to the V_{in} given in Eq. (28).

The induced dipole moment is defined by

$$\boldsymbol{P}(t)=\int\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\,|\phi(\boldsymbol{r}_0^{-1},t)|^2\,d\boldsymbol{r}_0^{-1}-\int\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\,|\Phi_1(\boldsymbol{r}_0^{-1})|^2\,d\boldsymbol{r}_0^{-1}, \tag{37}$$

where $\phi(\boldsymbol{r}_0^{-1},t)$ is determined by Eq. (10). The second term of Eq. (37) is always zero, provided the target atom is in the ground state. Making use of Eqs. (11) and (13), $\boldsymbol{P}(t)$ is represented by

$$\boldsymbol{P}(t)=2\,\mathrm{Re}\left[\sum_{n\neq1}^{\infty}(-i)\left\langle 1\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|n\right\rangle\int_{-\infty}^{t}dt_1V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}\right]. \tag{37-a}$$

Taking account of this expression, each term on the right hand side of Eq. (36) is reduced to

$$\frac{Z'\boldsymbol{P}(z)\cdot\boldsymbol{r}_0}{r_0^3}=2\,\mathrm{Re}\left[\sum_{n\neq1}^{\infty}(-i)\int_{-\infty}^{t}dt_1V_{1n}(t)V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}\right]+O(V^3), \tag{38}$$

and

$$-Z'\int_{-\infty}^{z}\frac{1}{r_1^3}\left\{\boldsymbol{r}_1\cdot\frac{d\boldsymbol{P}(z_1)}{dz_1}\right\}dz_1=\sum_{n\neq1}^{\infty}\omega_{n1}\left|-i\int_{-\infty}^{t}dt_1V_{n1}(t_1)e^{i\omega_{n1}t_1}\right|^2+O(V^3). \tag{39}$$

Inserting Eqs. (38) and (39) into Eq. (36), the latter is transformed into

$$W(\boldsymbol{r}_0)=2\,\mathrm{Re}\left[\sum_{n\neq1}^{\infty}(-i)\int_{-\infty}^{t}dt_1V_{1n}(t)V_{n1}(t_1)e^{-i\omega_{n1}(t-t_1)}\right]+\sum_{n\neq1}^{\infty}\omega_{n1}\left|-i\int_{-\infty}^{t}dt_1V_{n1}(t_1)e^{i\omega_{n1}t_1}\right|^2+O(V^3).$$

This is exactly the same as V_{in} Eq. (28). The same discussions as in § 3.2 can be made to define the polarization potential.

3.4. *Numerical Examples*

In order to see semi-quantitatively the dependence of the polarization potential on the incident velocity, we consider a hydrogen atom as the target and take into account only the first excited p state. This is because about 66% of the polarizability of hydrogen atom comes from this state as reported by Castillejo *et al.* [2].

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In §§ 2 and 3 we eventually defined two types of polarization potential. Equation (26) is derived from the second Born approximation and it is named "*nonadiabatic potential of type I*" in figures. Equation (28) is defined by the energy expectation value and is named "*nonadiabatic potential of type II*" in figures. Resulting potentials for $t<0$ are plotted in Fig. 2 and those for $t>0$ in Fig. 3. The value evaluated from Eq. (26) are shown by dots for some combinations of the incident velocity v and the impact parameter b (say inverted triangle ▼ for $v=0.10$ and $b=8$). The values of $v=0.10, 0.49$, and 4.9, correspond to the incident energy 0.3, 6.0, and 600 keV for incident protons, and correspond to 0.16, 3.26, and 326 eV for incident electrons, respectively. The values evaluated from Eq. (28) are represented by lines (say solid line —— for $v=0.10$ and $b=8$). The behavior of the calculated polarization potential in Fig. 2 agrees reasonably well with our expectation. That is, when the value of v/b is small, the polarization potential defined by Eqs. (26) and (28) is identical with the usual adiabatic polarization potential. As the value of v/b becomes large, the absolute magnitude of the polarization potential becomes smaller than the adiabatic one. These results reflect the difficulty of polarization of the target atom in faster encounter as compared with the case of adiabatic approach. The results in Fig. 3 contain an effect of excitations, because such contribution to the polarization potential defined by Eq. (28) has not been removed. When excitations occur, that is, the value of v/b is large, the values evaluated from Eq. (28) become positive. This is because the excitation energy or the first term of Eq. (28) dominantly contributes to the potential. These results tell us that the

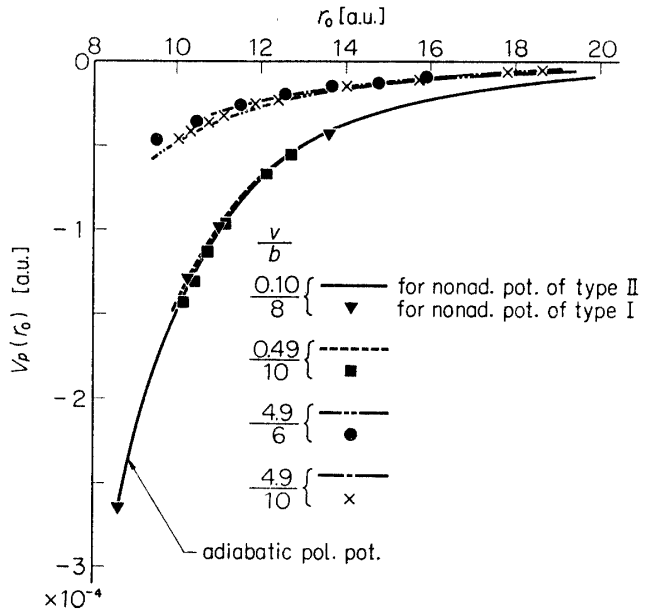

FIG. 2. Polarization potential given by Eqs. (26) and (28) before passing the point of the closest approach. Dots (say inverted triangle ▼ for $v=0.10$ and $b=8$) represent the results of the calculation of Eq. (26) named "nonadiabatic potential of type I", while lines (say solid lines —for $v=0.10$ and $b=8$) represent the results of Eq. (28) named "nonadiabatic potential of type II".

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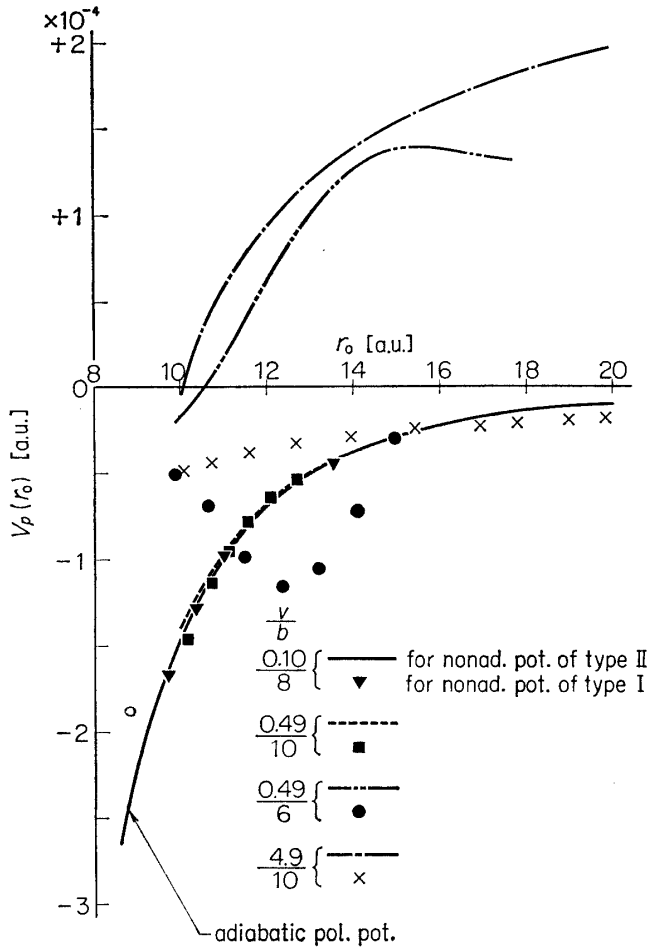

FIG. 3. Polarization potential given by Eqs. (26) and (28) after passing the point of the closest approach. Dots and lines are as in Fig. 2.

contribution of excitations to Eq. (28) must be removed to obtain the effective polarization potential for the elastic scattering. We take into account these and discuss the effective polarization potential in § 5.

4. Equivalence between the Induced Dipole Moment under Collision Processes and That Represented by the Dynamic Dipole Polarizability

In this section we confirm the equivalence of the induced dipole moment $\boldsymbol{P}(t)$ given by Eq. (37-a) with that derived by using the dynamic dipole polarizability. The following discussions are again limited within the validity of perturbation theory. We treat only the dipole polarization for simplicity, since dipole transitions will most easily take place. The generalization to other transitions will be straightforward. In the collision problems the interaction between the atom and the incident particle is written in the dipole approximation as follows

$$V(\boldsymbol{r}_0^{-1}, t) \cong -\sum_{i=1}^{Z} (-\boldsymbol{r}_i) \cdot \boldsymbol{F}(t), \tag{40}$$

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where

$$\boldsymbol{F}(t)=-\frac{Z'}{r_0(t)^2}\hat{\boldsymbol{r}}_0. \tag{40-a}$$

The induced dipole moment $\boldsymbol{P}(t)$ given by Eq. (37-a) is reduced to

$$\boldsymbol{P}(t)=2\,\mathrm{Re}\sum_{n\neq 1}^{\infty}\left\{i\int_{-\infty}^{t}dt_1\left\langle 1\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|n\right\rangle\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle\cdot\boldsymbol{F}(t_1)e^{-i\omega_{n1}(t-t_1)}\right\}. \tag{41}$$

When the time-dependent electric field $\boldsymbol{F}(t)$ is given, we can calculate the induced dipole moment $\boldsymbol{P}(t)$ in another way. Namely, the induced dipole moment, as shown by the following equation (44), is represented by the dynamic dipole polarizability. We first analyse the field $\boldsymbol{F}(t)$ into the Fourier component $\tilde{\boldsymbol{F}}(\omega)$ as follows

$$\boldsymbol{F}(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega e^{-i\omega t}\tilde{\boldsymbol{F}}(\omega), \tag{42-a}$$

and define the inverse transformation of this expression by

$$\tilde{\boldsymbol{F}}(\omega)=\int_{-\infty}^{\infty}dt e^{i\omega t}\boldsymbol{F}(t). \tag{42-b}$$

The dipole moment of the atom induced by the monochromatic wave $e^{-i\omega t}\tilde{\boldsymbol{F}}(\omega)$ is represented by

$$\tilde{\boldsymbol{P}}(\omega)e^{-i\omega t}=\tilde{\alpha}(\omega)\tilde{\boldsymbol{F}}(\omega)e^{-i\omega t}, \tag{43}$$

where $\tilde{\alpha}(\omega)$ is the dipole polarizability tensor of the atom defined by this equation, and is called the dynamic dipole polarizability tensor. Then the dipole moment $\boldsymbol{P}(t)$ as well as $\boldsymbol{F}(t)$ may be obtained as the superposition of the component induced by the monochromatic wave by

$$\boldsymbol{P}(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega e^{-i\omega t}\tilde{\boldsymbol{P}}(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega e^{-i\omega t}\tilde{\alpha}(\omega)\tilde{\boldsymbol{F}}(\omega). \tag{44}$$

We take here and hereafter the coordinate axis along the principal axes of the polarizability tensor.

The induced dipole moment defined by Eq. (37) should be equivalently represented by the dynamic dipole polarizability. We confirm this statement in the following. The dynamic dipole polarizability, as is well-known, is given by

$$\tilde{\alpha}(\omega)=\sum_{n\neq 1}^{\infty}\left\langle 1\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|n\right\rangle\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle\frac{2\omega_{n1}}{\omega_{n1}^2-\omega^2}, \tag{45}$$

where ω is not in the neighbourhood of any of excitation frequencies of atom. In integrating the right hand side of Eq. (44) the form of $\tilde{\alpha}(\omega)$ defined over all the value of ω is needed. To obtain such dynamic dipole polarizability (denoted by $\tilde{\alpha}_e(\omega)$), we

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take into account the finite breadth of excited states of atom as $\{E_n-(i\Gamma_n/2)\}$ for $n\neq 1$ and $\Gamma_1\equiv 0$. The required form is obtained as follows

$$\tilde{\alpha}_e(\omega)=\sum_{n\neq 1}^{\infty}\frac{\left\langle 1\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|n\right\rangle\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle}{\omega_{n1}-\omega-i\Gamma_n/2}. \tag{46}$$

The usual dynamic dipole polarizability is given by

$$\lim_{\Gamma_n\to 0}(\tilde{\alpha}_e(\omega)+\tilde{\alpha}_e(-\omega)). \tag{46-a}$$

Inserting Eqs. (42–b) and (46) into the right hand side of Eq. (44), and integrating with respect to ω, we obtain the expression of $\boldsymbol{P}(t)$ as follows

$$\boldsymbol{P}(t)=2\,\mathrm{Re}\left[\sum_{n\neq 1}^{\infty} i\int_{-\infty}^{t}dt_1\left\langle 1\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|n\right\rangle\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle \cdot\boldsymbol{F}(t_1)e^{\{-i(\omega_{n1}+(Im\,\Gamma_n/2))-(\mathrm{Re}\,\Gamma_n/2)\}(t-t_1)}\right]. \tag{44-a}$$

To make the expression (44) fit the real dipole moment as the response to the real perturbation force, we take here twice the real part of Eq. (44). The contribution to the integration of Eq. (44-a) mainly comes from the time interval shorter than the life time of excited states of atom. In general, the life time of excited states of atom is very long as compared with the collision time. For example, the life time of the $2P_{3/2}$ for hydrogen atom, as shown by Heitler [*19*], is about 6.5×10^9 a.u., and the collision time is the order of several atomic unit even for incident protons with energy of several hundred eV in the case of distant collisions. We may neglect the factor $\exp[(-(\mathrm{Re}\,\Gamma_n/2)-i(\mathrm{Im}\,\Gamma_n/2))(t-t_1)]$ in the integrand of Eq. (44–a). We obtain the induced dipole moment as

$$\boldsymbol{P}(t)=2\,\mathrm{Re}\sum_{n\neq 1}^{\infty}\left\{i\int_{-\infty}^{t}dt_1\left\langle 1\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|n\right\rangle\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle\cdot\boldsymbol{F}(t_1)e^{-i\omega_{n1}(t-t_1)}\right\}. \tag{47}$$

This is the same as Eq. (41). Thus the induced dipole moment $\boldsymbol{P}(t)$ under collision processes is represented by the dynamic dipole polarizability which has been investigated previously in detail. As shown in § 3. 3, we are able to obtain approximately the dynamic polarization potential from the information of the dynamic polarizability [*20*].

When the real excitations occur, the induced dipole and multipole moments of the target oscillate with the finite amplitudes even after the collision. This is seen, for example, from the asymptotic forms Eqs. (22-c) and (22-d) of the induced dipole moment Eq. (37-a) for a hydrogen atom as the target atom. We are able to know the excitation probability from the magnitudes of the induced dipole and multipole moments. The induced dipole and multipole moments, as is shown above, are represented by the dynamic polarizability. Thus the excitation probability may be inferred by making use of the dynamic polarizability. We shall again confine our discussions to dipole transitions. The excitation probability, to the

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first approximation, is given by Eq. (13). By adopting the dipole approximation Eqs. (40) and (40-a) and using Eq. (42-a), the probability amplitude of excitation is given by

$$C_n^{(1)}(\infty)=\frac{i}{2\pi}\int_{-\infty}^{\infty}dt_1\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle\cdot\int_{-\infty}^{\infty}d\omega\tilde{\boldsymbol{F}}(\omega)e^{-i(\omega-\omega_{n1})t_1},$$
$$=i\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle\cdot\tilde{\boldsymbol{F}}(\omega_{n1}). \tag{48}$$

Here we change the order of integration with respect to time t and the one with respect to frequency ω and make use of the well-known relation of δ-function. As the dynamic dipole polarizability, as seen from Eq. (46), has the remarkable value near the excitation frequency $\omega\cong\omega_{n1}$, the square of the matrix element $|\langle n|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)|1\rangle|^2$ may be expressed by

$$\left|\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle\right|^2=\frac{1}{2}\left[\lim_{\omega\to(\omega_{n1}-(\mathrm{Im}\Gamma_n/2))}\left(\omega_{n1}-\frac{i\Gamma_n}{2}-\omega\right)\tilde{\alpha}_e(\omega)\right.$$
$$\left.+\lim_{\omega\to-(\omega_{n1}-(\mathrm{Im}\Gamma_n/2))}\left(\omega_{n1}-\frac{i\Gamma_n}{2}+\omega\right)\tilde{\alpha}_e(-\omega)\right]. \tag{49}$$

The dynamic polarizability having a physical meaning is a real quantity, and the relation $\mathrm{Re}\,\tilde{\alpha}_e(-\omega)=\mathrm{Re}\,\tilde{\alpha}_e(\omega)$, in general, holds. Furthermore, the level shifts of the excited states of atom are fairly small as compared with the level intervals of the atom. Equation (49) may be approximated by

$$\left|\left\langle n\left|\sum_{i=1}^{Z}(-\boldsymbol{r}_i)\right|1\right\rangle\right|^2\cong\lim_{\omega\to\omega_{n1}}(\omega_{n1}-\omega)\,\mathrm{Re}\,\tilde{\alpha}_e(\omega). \tag{49-a}$$

Using Eqs. (48) and (49–a), we obtain the excitation probability as follows

$$|C_n^{(1)}(\infty)|^2=\lim_{\omega\to\omega_{n1}}(\omega_{n1}-\omega)\,\mathrm{Re}\,\tilde{\alpha}_e(\omega)\,|\tilde{\boldsymbol{F}}(\omega_{n1})|^2, \tag{50}$$

where $\tilde{\boldsymbol{F}}(\omega_{n1})$ is represented by Eqs. (7), (40—a), and (42–b). Thus we are able to estimate the excitation cross section of a neutral atom by a charged particle impact, provided the dynamic dipole polarizability of the atom is known with a sufficient accuracy in the neighbourhood of ω_{n1}.

5. Discussions

We have defined the polarization potential in §§ 2 and 3 by Eq. (6) (the real part of Eq. (6) is denoted by V_p^{I}) and in § 3 by Eqs. (27) or (28) for sufficiently low incident energy (denoted by V_p^{II}). Unfortunately, they are not identical to each other. Which definition is more appropriate for the polarization potential? The complex polarization potential Eq. (6) is defined as an effective potential in the scattering equation (4), and has an imaginary part. Such imaginary term must not be contained in the effective polarization potential for the elastic scattering. When

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the incident energy is sufficiently high, the asymptotic form of V_p^{I} is given by Eq. (23). As mentioned just under Eq.(23), it is positive for the scattering angle θ for which $\cos\theta > 1/3$. This peculiar behavior only holds in the case of $k_n \cong k_1$, and disappears as the incident energy decreases. In the intermediate energy region the asymptotic form of V_p^{I} is given by Eqs. (22) and (22-a~d). As seen from Eq. (27), we do not know the role that the V_p^{II} plays in the scattering problem. The asymptotic form of V_p^{II}, Eq. (32), is derived from Eq. (28) in the limit of $t \to -\infty$ for an intermediate incident energy. In the limit of $t \to +\infty$ the excitation energy, the permanent dipole interaction, Eq. (22-b), multiplied by 2, and so forth are added to Eq. (32). In the adiabatic limit both definitions Eqs. (6) and (27) are identical to each other. When the real excitations occur, both V_p^{I} and V_p^{II} contain the effect of excitations as is noted above. In the short and intermediate distances from the origin, we can not separate such effect into the part contributing to the elastic channel and the others. Both this fact and the ambiguity included in the scattered wave function mentioned in the Introduction prevent us from uniquely defining the polarization potential. The asymptotic forms Eqs. (22) and (32) in the limit of $t \to -\infty$ agree with each other except the numerical factor in the second term of their expressions. The difference of numerical factor comes from the distinction between definitions of the polarization potential. It is unable to decide that one of V_p^{I} and V_p^{II} is more suitable than the other as the effective polarization potential.

We thus infer the effective polarization potential for the elastic scattering on the basis of the asymptotic forms Eqs. (22) and (32). We adopt as the asymptotic form

$$V_p(r) \sim -\frac{\alpha Z'^2}{2r^4}\left(1-\frac{av^2}{\omega^2 r^2}\right)+O\left(\frac{1}{r^7}\right), \tag{32-a}$$

where a is 6 for V_p^{I}, and 4 for V_p^{II}. The correction term for the adiabatic potential explicitly depends on the incident velocity. The dependence of the polarization potential on the incident velocity was shown by Garrett [11], but a drastic approximation introduced in the course of his calculations is hard to be admitted. The behavior of the correction term as $1/r^6$ has been obtained by several works [3, 4, 5, 6], but all of their correction terms does not depend on the incident velocity. The character of the correction terms of this work and that of works just mentioned are quite different. Castillejo *et al.* [2] have concluded that in the asymptotic region the polarization potential which behaves $(-\alpha/2r^4)$ is independent of the velocity of the incident electron, so long as it is insufficient to excite the atom. But Eq. (32-a) does not contradict with their conclusion to the order of $1/r^5$.

The factor in Eq. (32-a), $\{1-(av^2/\omega^2 r^2)\}$, is equal to the first two terms of the Taylor expansion of some functions, say $\exp(-av^2/\omega^2 r^2)$ or $1/\{1+(av^2/\omega^2 r^2)\}$. Thus we first propose the following two expressions as the effective polarization potential over wide range of the incident energy

$$V_p(r) = V_{ad.p}(r) e^{-(av^2/\omega^2 r^2)}, \tag{51-a}$$

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and

$$V_p(r)=V_{ad.p}(r)\left(1+\frac{av^2}{\omega^2 r^2}\right)^{-1}, \tag{51-b}$$

where $V_{ad.p}(r)$ is the usual adiabatic polarization potential. The values evaluated from Eqs. (28), (51–a) and (51–b) are plotted in Fig. 4. The ratios of the values of Eq. (51–b) to those of Eq. (28) vary from about 1.0 to 0.4, and those of Eq. (51–a) to Eq. (28) extend from about 1.0 to 0.001, when v/b increases from 0.49/10 to 4.9/6. In evaluating Eqs. (51–a) and (51–b) we choose ω_{21} as the value of ω and $a=4$. If the value of ω is larger than ω_{21}, the differences between the values of Eqs. (28) and (51–a) and those of Eqs. (28) and (51–b) become somewhat smaller, but much improvement is not expected. Then we compare the values of Eq. (28) with those of the expressions for $a=1$ in Eqs. (51–a) and (51–b). The results are plotted in Fig. 5. The difference between these values and those of Eq. (28) are within 20 percents, even if v/b increases from 0.49/10 to 4.9/6. As seen from these

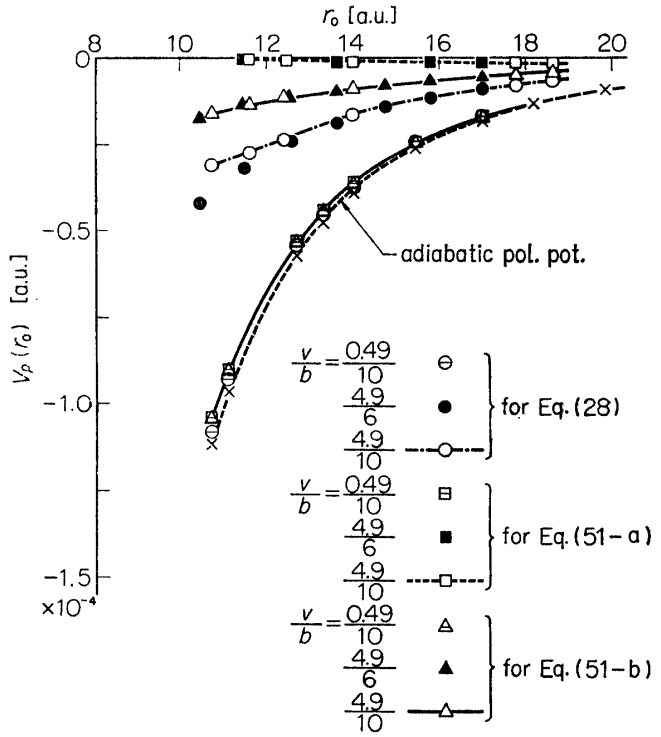

FIG. 4. Comparison between the polarization potential given by Eq. (28) and those given by Eqs. (51–a) and (51–b). The broken line represents the adiabatic polarization potential, the dash-dotted lines the polarization potential given by Eq. (28), the dotted lines that given by Eq. (51–a), and the solid lines that given by Eq. (51–b). Here a and ω are chosen 4 and ω_{21}, respectively. For the combination of $v=0.49$ and $b=10$, the values calculated from Eqs. (51–a) and (51–b) are almost coincident. We are able to make no difference between them and the values evaluated from Eq. (28) for $r_0 \geq 15$ a.u.

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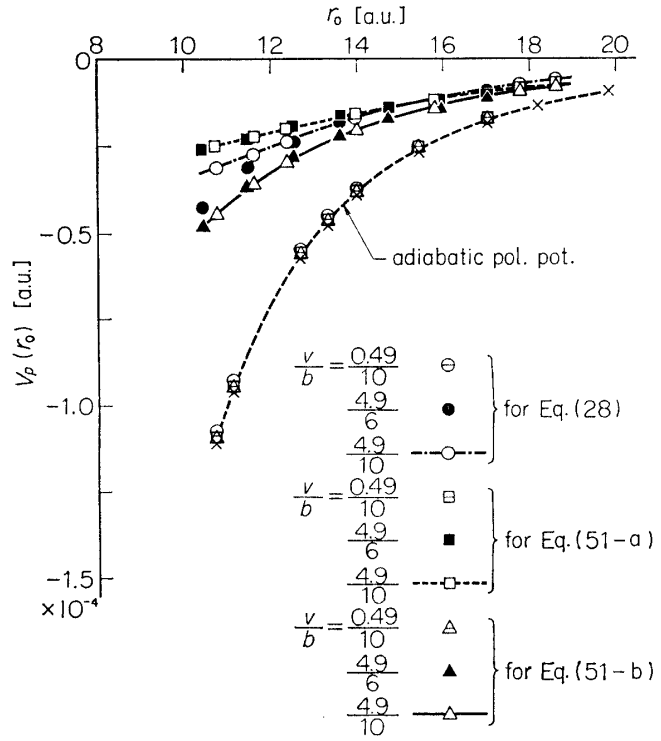

FIG. 5. Comparison between the polarization potential given by Eq. (28) and those given by Eqs. (51-a) and (51-b). Here a and ω are chosen 1 and ω_{21}, respectively. For the combination of $v=0.49$ and $b=10$, the values calculated from Eqs. (51-a) and (51-b) are coincident. We are able to make no difference between them and the values evaluated from Eq. (28) for $r_0 \geq 15$ a.u.

results, the nonadiabatic potential with the factor $\exp(-av^2/\omega^2 r^2)$ as the correction terms for the adiabatic potential is much more sensitively dependent on the numerical factor a than that with the factor $\{1+(av^2/\omega^2 r^2)\}^{-1}$. Thus we propose as the form of the effective polarization potential for the elastic scattering

$$V_p(r)=V_{ad.p}(r)\left(1+\frac{v^2}{\omega^2 r^2}\right)^{-1}, \tag{52}$$

or

$$V_p(r)=V_{ad.p}(r)\left(1+\frac{k_1^2}{\mu_0^2\omega^2 r^2}\right)^{-1}. \tag{53}$$

Here ω is an average excitation energy, but it may be regarded as a parameter to be suitably chosen. One way by which ω is determined is that we make the differential cross section evaluated with the form of Eqs. (52) or (53) as polarization potential fit the experimental value at any incident energy. The form of Eqs. (52) or (53), instead the polarization potential investigated thus far, well represents the physical situation. As the incident velocity v becomes large within the restriction $(v/\omega)<r$, the target atom is less polarized. Thus the polarization potential

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becomes smaller, as the velocity of incident particle increases.

In obtaining Eqs. (52) or (53), we confine ourselves to the discussions in the distant collisions, and make the assumptions, that is, both the perturbation theory and the dipole approximation are applicable. The proposition Eqs. (52) or (53) with ω as determined above will be useful for discussing the differential cross sections, in particular in the small angle scattering, of the elastic scattering, provided the limitation and assumptions do not cause much error in the problem considered. Its validity may be tested by applying to real problems.

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