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# Coulomb effects in the interaction of a charged particle with a two-fragment quantum system

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**Abstract.** A direct method to derive the expression for the polarization potential between a charged particle and a two-fragment quantum system is developed. This method is based on the asymptotic properties of the two-body Coulomb Green function. The explicit form of the polarization potential constant is obtained for low-energy deuteron–nucleus scattering and for ion–hydrogen scattering. The properties of the polarization potential at high collision energies are applied to obtain an expression for the ion–atom scattering total cross section.

## 1. Introduction

The investigation of Coulomb scattering involving many-particle quantum systems is of great importance in atomic, molecular, and nuclear physics. In particular, the investigation of the behaviour of the two-fragment system in an external Coulomb field is an effective method to study its internal structure. In the general case, the particles, produced in the reaction simultaneously with the system under consideration, act as the field sources. For stable quantum systems the potential corresponding to its interaction with an external Coulomb point-like source can be represented as a sum of the pure Coulomb term, an additional multipole-type potential, and the polarization potential. The properties of the polarization interaction have been considered extensively in the past (see, for example [1–4]).

In this paper we consider the problem of derivation of the polarization potential on the basis of rigorous many-particle scattering theory. We formulate a direct method for obtaining the expression for this potential for Coulomb scattering of a charged particle by a two-fragment bound system. Our approach is based on the asymptotic properties of the two-body Coulomb Green function and the results obtained taking account of the effects of non-zero collision energy, thus exceeding the applicability of the adiabatic approximation [1, 2]. Furthermore, the method developed can be generalized for the description of the external force field influence on the observable properties of unstable quantum systems in nuclear and atomic physics [5–8].

The foundations of the theory are presented in section 2, while applications to both low- and high-energy scattering in various systems is shown in section 3. The atomic system of units is used throughout the text except where noted.

## 2. Theory

The Hamiltonian that characterizes the three-body problem under investigation can be represented as [9]

$$H = H_\alpha + V^\alpha \quad (1)$$

where the index  $\alpha$  denotes the two-fragment bound system and  $V^\alpha$  is the Coulomb potential of the third particle with the fragments which form the pair  $\alpha$ . The channel Hamiltonian  $H_\alpha$  is given by the expression

$$H_\alpha = \tilde{H}_\alpha + h_{0\alpha} \quad (2)$$

where  $\tilde{H}_\alpha$  is the Hamiltonian of internal motion in the subsystem  $\alpha$  and  $h_{0\alpha}$  is the free Hamiltonian of relative motion of  $\alpha$  and the third particle. The operator  $H$  can then be represented as

$$H = \tilde{H}_\alpha + (h_{0\alpha} + V_c^\alpha) + W^\alpha = \tilde{H}_\alpha + h_\alpha^c + W^\alpha \quad (3)$$

where  $V_c^\alpha$  is the Coulomb potential between the pair  $\alpha$  (considered here as a point particle) and the third particle,  $h_\alpha^c = h_{0\alpha} + V_c^\alpha$  is the Hamiltonian of the subsystem  $\alpha$  in the field of the third particle and  $W^\alpha = V^\alpha - V_c^\alpha$  is the potential responsible for the polarization effects.

We define an operator  $\mathcal{P}$  as a projection operator onto the bound states of the internal motion Hamiltonian  $\tilde{H}_\alpha$  with the energy  $-\kappa^2$  and the total spin  $j$  (i.e.  $\mathcal{P} = \sum_m |\phi_{jm}\rangle \langle \phi_{jm}|$ ). Then the optical potential (e.g. the effective interaction potential) for the pair  $\alpha$ -third particle follows in the form [9–11]

$$\begin{aligned} U_{mm'}(\mathcal{Z}) &= \langle \phi_{jm} | W^\alpha + W^\alpha R(\mathcal{Z}) W^\alpha | \phi_{jm'} \rangle \\ &= \langle \phi_{jm} | W^\alpha [I - \hat{g}_\alpha(\mathcal{Z} - h_\alpha^c) W^\alpha]^{-1} | \phi_{jm'} \rangle \end{aligned} \quad (4)$$

where  $\mathcal{Z} = E + i0$  is the total energy of the three-body system. In the derivation of formula (4) we have used the convolution of the Green function for the subsystem and the Coulomb Green function  $g_\alpha^c(\mathcal{Z})$  [12]

$$\tilde{G}_\alpha(\mathcal{Z}) = \int_{-\infty}^{\infty} \frac{d\epsilon}{-2i\pi} g_\alpha(\epsilon + i0) \otimes g_\alpha^c(\mathcal{Z} - \epsilon) \quad (\text{Im } \mathcal{Z} > 0) \quad (5)$$

with the following designations

$$\tilde{G}_\alpha(\mathcal{Z}) = (\mathcal{Z} - \tilde{H}_\alpha - h_\alpha^c)^{-1} \quad (6)$$

$$g_\alpha^c(\mathcal{Z}) = (\mathcal{Z} - h_\alpha^c)^{-1} \quad (7)$$

$$g_\alpha(\mathcal{Z}) = (\mathcal{Z} - \tilde{H}_\alpha)^{-1} \quad (8)$$

and where the symbol  $\otimes$  denotes the tensor product.

Using the spectral theorem for the resolvent operator  $g_\alpha^c(\mathcal{Z})$  we express the operator  $\tilde{G}_\alpha(\mathcal{Z})$  in the form

$$\tilde{G}_\alpha(\mathcal{Z}) = g_\alpha(\mathcal{Z} - h_\alpha^c). \quad (9)$$

Since the operator  $R(\mathcal{Z})$  in (4) satisfies the equation

$$R(\mathcal{Z}) = \hat{g}_\alpha(\mathcal{Z} - h_\alpha^c) + \hat{g}_\alpha(\mathcal{Z} - h_\alpha^c) W^\alpha R(\mathcal{Z}) \quad (10)$$

with  $\hat{g}_\alpha(\mathcal{Z}) = g_\alpha(\mathcal{Z})(I - \mathcal{P})$ ,  $R(\mathcal{Z})$  is the resolvent of the Hamiltonian  $H$  in the orthogonal subspace, defined by the projection operator  $\mathcal{Q} = I - \mathcal{P}$  [9–11]

$$R(\mathcal{Z}) = (\mathcal{Z}\mathcal{Q} - \mathcal{Q}H\mathcal{Q})^{-1}\mathcal{Q}. \quad (11)$$

The solution of the integral equation (10) may be obtained by iterations, thus yielding the following expression for the effective potential

$$\begin{aligned} U_{mm'}(\mathcal{Z}) &= \langle \phi_{jm} | W^\alpha | \phi_{jm'} \rangle + \langle \phi_{jm} | W^\alpha \hat{g}_\alpha(\mathcal{Z} - h_\alpha^c) W^\alpha | \phi_{jm'} \rangle + \dots \\ &= \sum_n U_{mm'}^{(n)}(\mathcal{Z}). \end{aligned} \quad (12)$$

The first term  $U_{mm'}^{(1)}(\mathcal{Z})$  in equation (12) corresponds to the effective potential in the Born approximation. In the coordinate representation this term is local and diverges exponentially when  $\rho \rightarrow 0$  (the total angular momentum of the pair  $\alpha$  equals 0) or as  $\rho^{-3}$  (the total pair  $\alpha$  angular momentum differs from 0) [4–13], where  $\rho$  is the distance between the charge and the centre-of-mass of the two-fragment system. Addition of the pure Coulomb term  $V_\alpha^c$  to  $U_{mm'}^{(1)}(\mathcal{Z})$  gives the static part of the interaction potential

$$V^{\text{st}} = V_\alpha^c \delta_{mm'} + U_{mm'}^{(1)} = \langle \phi_{jm} | V^\alpha | \phi_{jm'} \rangle. \quad (13)$$

The decomposition equation (13) is the starting point of Veselova's regularization procedure in the integral equations for three charged particles [13, 14].

The second term in equation (12) corresponds to the polarization potential and has the form

$$\langle \rho | \langle \phi_{jm} | W^\alpha \hat{g}_\alpha(\mathcal{Z} - h_\alpha^c) W^\alpha | \phi_{jm'} \rangle | \rho' \rangle. \quad (14)$$

Using the convolution form of  $\hat{g}_\alpha(\mathcal{Z} - h_\alpha^c)$  in equation (5) we conclude that the asymptotic behaviour  $\langle \rho | U_{mm'}^{(1)} | \rho' \rangle$  is defined by the asymptotic properties of the two-body Coulomb Green function  $g_c(\mathcal{Z})$ .

To describe these asymptotic properties we use the partial-wave expansion of the Coulomb Green function [10]

$$\langle \rho | g_c(\mathcal{Z}) | \rho' \rangle = \frac{2\mu}{\rho\rho'} \sum_{\ell\lambda} Y_{\ell\lambda}(\rho) Y_{\ell\lambda}^*(\rho') g_c^\ell(\rho, \rho', \mathcal{Z}) \quad (15)$$

where  $k = (2\mu\mathcal{Z})^{1/2}$ ,  $\mu$  being the two-body reduced mass,  $\mu = \frac{m_1 m_2}{m_1 + m_2}$  and

$$\begin{aligned} g_c^\ell(\rho, \rho', \mathcal{Z}) &= i(-1)^\ell (4k^2 \rho \rho')^{\ell+1} \frac{\Gamma(\ell + 1 + i\eta)}{(2\ell + 1)!} \exp(ik(\rho + \rho')) \frac{1}{2k} \\ &\times \Phi(\ell + 1 + i\eta, 2\ell + 2, -2ik\rho_<) \Psi(\ell + 1 + i\eta, 2\ell + 2, -2ik\rho_>). \end{aligned} \quad (16)$$

As usual,  $\rho_<$  and  $\rho_>$  are the smaller and larger of  $\rho$  and  $\rho'$ , respectively, and  $\eta$  is the Coulomb parameter  $\eta = \frac{Q_1 Q_2 \mu}{k}$ , where  $Q_1$  and  $Q_2$  are the charges of the particles. In the asymptotic region  $|k\rho| \gg 1$ ,  $|k\rho'| \gg 1$  the partial Green function  $g_c^\ell(\rho, \rho', \mathcal{Z})$  contains a contribution of the form

$$-\frac{1}{2} \left( \frac{\rho_<}{\rho_>} \right)^{i\eta} \exp(ik(\rho_> - \rho_<)). \quad (17)$$

We note that such a contribution, containing the exponent  $\exp(ik(\rho + \rho'))$ , introduces terms into  $\langle \rho | U_{mm'}^{(2)} | \rho' \rangle$  of an asymptotically higher order than those in equation (17) and thus this contribution can be omitted. Therefore,

$$\langle \rho | g_c(\mathcal{Z}) | \rho' \rangle \mapsto \frac{\mu}{ik} \frac{1}{\rho\rho'} \left( \frac{\rho_<}{\rho_>} \right)^{i\eta} \exp(ik(\rho_> - \rho_<)) \delta(\Omega_\rho - \Omega_{\rho'}) \quad (18)$$

when  $|k\rho| \gg 1$ ,  $|k\rho'| \gg 1$  and

$$\langle \rho | g_c(\mathcal{Z}) | f \rangle \mapsto \frac{\mu}{ik} \rho \int_0^\infty dx x^{1+i\eta} \exp(ik\rho|1-x|) f(x\rho, \Omega_\rho) \quad (19)$$

if  $|k\rho| \gg 1$ .  $f(\rho)$  is a smooth function, significantly different from zero only at large distances  $\rho$ . Using standard asymptotic methods, we find the asymptotic expression for equation (19):

$$\langle \rho | g_c(\mathcal{Z}) | f \rangle \mapsto \frac{2\mu}{k^2} f(\rho) \quad (20)$$

which is valid when  $|k\rho| \gg 1$ . Equation (20) implies that

$$\langle \rho | g_c(\mathcal{Z}) | \rho' \rangle \mapsto \frac{2\mu}{k^2} \delta(\rho - \rho') = \frac{1}{\mathcal{Z}} \delta(\rho - \rho') \quad (21)$$

when both  $|k\rho| \gg 1$  and  $|k\rho'| \gg 1$ .

The result obtained opens the possibility to calculate the matrix elements of the polarization potential  $\langle f | V_{\text{pol}}(\mathcal{Z}) | f' \rangle$  with functions  $f(\rho)$  and  $f'(\rho)$  smoothly vanishing at small distances. The kernel of  $V_{\text{pol}}(\mathcal{Z})$  is obtained in this case by substitution of equation (21) into equation (14). In the dipole approximation for  $W^\alpha$  we find that

$$\begin{aligned} \langle \rho | U_{mm'}^{(2)} | \rho' \rangle &= \frac{1}{\rho^2 \rho'^2} \int_{-\infty}^{\infty} \frac{d\epsilon}{-2i\pi} \int d\mathbf{r} \int d\mathbf{r}' r r' C^2 \psi_m^*(\mathbf{r}) \cos(\mathbf{r}, \rho) \tilde{\theta}(\rho - r) \\ &\quad \times \langle \mathbf{r} | \hat{g}_\alpha(\epsilon + i0) | \mathbf{r}' \rangle \cos(\mathbf{r}', \rho') \tilde{\theta}(\rho' - r') \psi_{m'}(\mathbf{r}') \langle \rho | g_\alpha^c(\mathcal{Z} - \epsilon) | \rho' \rangle. \end{aligned} \quad (22)$$

The terms containing the step functions  $\tilde{\theta}(r - \rho)$  or  $\tilde{\theta}(r' - \rho')$  ( $r$  being the relative coordinate in the pair  $\alpha$ ) are exponentially small and we replace the sharp cut-off  $\tilde{\theta}(\rho - r)$  by the smooth one  $(1 + \exp((r - \rho)/a))^{-1}$ . Assuming that the Hamiltonian  $\hat{H}_\alpha$  is analytical under complex scaling [13, 16, 17] (and thus the function  $\psi_m(r) = (1 + \exp((r - \rho)/a))^{-1} \phi_m(r)$  is an analytical vector [16]), we can rewrite equation (22) as

$$\begin{aligned} \langle \rho | U_{mm'}^{(2)} | \rho' \rangle &= \frac{1}{\rho^2 \rho'^2} C^2 \int_{-\infty}^{\infty} \frac{d\epsilon}{-2i\pi} \int d\mathbf{r} \int d\mathbf{r}' r r' \phi_m^*(e^{\theta*} \mathbf{r}) \cos(\mathbf{r}, \rho) \langle \mathbf{r} | \hat{g}_\alpha^\theta(\epsilon + i0) | \mathbf{r}' \rangle \\ &\quad \times \cos(\mathbf{r}', \rho') \phi_{m'}(\mathbf{r}') \langle \rho | g_\alpha^c(\mathcal{Z} - \epsilon) | \rho' \rangle \end{aligned} \quad (23)$$

where we have used the second Balslev–Combes theorem [15, 16]

$$\langle \Psi_m | \hat{g}(\epsilon + i0) | \Psi_{m'} \rangle = \langle \Psi_m(\theta^*) | \hat{g}_\alpha^\theta(\epsilon + i0) | \Psi_{m'}(\theta) \rangle \quad (24)$$

and  $\theta$  is a complex scaling parameter, not to be confused with the step function  $\tilde{\theta}(x)$ . The constant  $C$  in equations (22) and (23) is defined by the expression

$$C = Q_3 \frac{Q_2 m_1 - Q_1 m_2}{m_1 + m_2}. \quad (25)$$

Inserting the spectral representation for the  $\hat{g}_\alpha^\theta(\epsilon + i0)$  into equation (23) and assuming for simplicity that the Hamiltonian  $\mathcal{Q}H_\alpha\mathcal{Q}$  does not have a discrete spectrum, we reduce equation (23) to the form

$$\begin{aligned} &\int d\mathbf{q}_\alpha |\psi_\alpha^\theta(\mathbf{q})\rangle \langle \psi_\alpha^{\theta*}(\mathbf{q}_\alpha) | \times \langle \rho | g_c \left( \mathcal{Z} - e^{-2\theta} \frac{q_\alpha^2}{2\mu_\alpha} \right) | \rho' \rangle \\ &\quad + \sum |\psi_i(\theta)\rangle \langle \psi_i(\theta^*) | \times \langle \rho | g_c(\mathcal{Z} - \lambda_i) | \rho' \rangle \end{aligned} \quad (26)$$

where  $\int d\mathbf{q}_\alpha |\psi_\alpha^\theta(\mathbf{q})\rangle \langle \psi_\alpha^{\theta*}(\mathbf{q}_\alpha) |$  is the spectral projection operator onto the continuous spectrum of  $\mathcal{Q}H_\alpha\mathcal{Q}$  and where  $|\psi_i(\theta)\rangle$  is the resonant wavefunction for the pair  $\alpha$ , i.e.

$$\hat{H}_\alpha |\psi_i(\theta)\rangle = \lambda_i |\psi_i(\theta)\rangle. \quad (27)$$

Since

$$|k^\theta| = \left| \left( 2\mu_\alpha \left( \mathcal{Z} - e^{-2\theta} \frac{q_\alpha^2}{2\mu} \right) \right)^{1/2} \right| \neq 0 \quad (28)$$

where  $\mathcal{Z} \neq 0$  for arbitrary  $q_\alpha$  ( $\text{Im } \theta > 0$ ) and where  $\mu_\alpha = \frac{(m_1+m_2)m_3}{m_1+m_2+m_3}$  is the reduced mass of the pair  $\alpha$  plus the third particle, the result in equation (21) can be applied in equation (23). Using the limiting procedure  $\theta \mapsto 0$  in the resulting expression, we find

$$\begin{aligned} \langle \rho | U_{mm'}^{(2)} | \rho' \rangle &= \delta(\rho - \rho') \frac{C^2}{\rho^4} \int d\mathbf{r} \int d\mathbf{r}' \psi_m^*(\mathbf{r}) r \tilde{\theta}(\rho - r) \\ &\quad \times \cos(\mathbf{r}, \rho) \langle \mathbf{r} | \hat{g}_\alpha(\mathcal{Z}) | \mathbf{r}' \rangle r' \tilde{\theta}(\rho' - r') \cos(\mathbf{r}', \rho') \psi_{m'}(\mathbf{r}'). \end{aligned} \quad (29)$$

If we neglect the exponentially small corrections again, the final expression for the polarization potential follows in the form

$$\langle \rho | V_{\text{pol}}^{mm'}(\mathcal{Z}) | \rho' \rangle = \langle \rho | U_{mm'}^{(2)} | \rho' \rangle = -\frac{\gamma \delta(\rho - \rho')}{\rho^4} \quad (30)$$

where

$$\gamma = -C^2 \int d\mathbf{r} \int d\mathbf{r}' \psi_m^*(\mathbf{r}) r \cos(\mathbf{r}, \rho) \langle \mathbf{r} | \hat{g}_\alpha(\mathcal{Z}) | \mathbf{r}' \rangle r' \cos(\mathbf{r}', \rho') \psi_{m'}(\mathbf{r}'). \quad (31)$$

The result in equation (30) is valid for all  $\mathcal{Z} \neq 0$  and  $\mathcal{Z} \notin \sigma_d(H_{0\alpha} + V_\alpha)$  with the exception of the eigenvalue  $-\kappa_\alpha^2$  under consideration. Generally, for the negative energies of the system (particularly at the energies between the ground and the first excited state) the expressions in equation (30) coincide with the well known expression for the polarization potential in the adiabatic approximation. The approach developed here allows the validity of equation (30) to be extended for arbitrary energies,  $E$ . The exceptions are the threshold energies of the Hamiltonian  $\mathcal{Q}H_\alpha\mathcal{Q}$  and the region of relative distances  $\rho$  for which  $(2\mu_\alpha|\delta|)^{1/2}\rho \gg 1$ , where  $\delta$  is the distance from  $E$  to the nearest threshold.

As mentioned above, the result obtained relates to the properties of the kernel  $\langle \rho | V_{\text{pol}}(\mathcal{Z}) | \rho' \rangle$ . If the momenta  $\mathbf{p}$  and  $\mathbf{p}'$  obey the inequality  $p, p' \ll |\sqrt{2\mu_\alpha E}|$  it is easy to see that this result extends to the momentum space matrix elements  $\langle \mathbf{p} | V_{\text{pol}}(\mathcal{Z}) | \mathbf{p}' \rangle$  which describe the properties of the long-range part of the operator  $U_{mm'}^{(2)}(\mathcal{Z})$ .

### 3. Applications

#### 3.1. Deuteron–nucleus scattering

As a first example we derive the expression for the polarization potential corresponding to the low-energy scattering of the deuteron by the nucleus with charge  $Q = Q_3$ . Assuming that the nucleon–nucleon forces are described by a separable potential with the form factor in the Yukawa form (Yamaguchi potential) and using for simplicity the zero-range approximation we obtain

$$\langle \rho | V_{\text{pol}}(\mathcal{Z}) | \rho' \rangle = -\frac{\gamma \delta(\rho - \rho')}{\rho^4} \quad (32)$$

where

$$\gamma = \frac{Q^2 M_N}{64 \beta^4} {}_2F_1 \left( 1, \frac{5}{2}; 5; \frac{E_d^c + i0}{|\epsilon_b|} \right). \quad (33)$$

$E_d^c$  is the energy of the system (in the centre-of-mass),  $\epsilon_b = -\frac{\beta^2}{M_N}$  is the bound energy of the deuteron of reduced mass  $M_N$  and  ${}_2F_1$  is the hypergeometric function of the form

$${}_2F_1 \left( 1, \frac{5}{2}; 5; z \right) = \frac{4!16}{9z^4} \left[ (1-z)^{3/2} - 1 + \frac{3}{2}z - \frac{3}{8}z^2 - \frac{1}{16}z^3 \right]. \quad (34)$$

In the range of low energies, which is our current interest, one may assume  $E_d^c \cong 0$ , and the result obtained coincides with that obtained in [3].

### 3.2. Ion-hydrogen scattering

As a second example we calculate the polarization potential constant for the scattering of an ion of charge  $Q = Q_3$  by the hydrogen atom. Using the dipole approximation for the potential  $W(\rho)$  we obtain

$$\gamma = -\frac{4}{3}Q^2I \quad (35)$$

where

$$I = -\int_0^\infty dr \int_0^\infty dr' e^{-\beta(r+r')} r^2 r'^2 g_c^{\ell=1}(r, r', \mathcal{Z}) \quad (36)$$

and  $\beta = 1$  in case of the hydrogen ion.

To calculate the integral in equation (36) we use the following representation for the two-body Coulomb Green function [17]

$$g_c(\mathbf{r}, \mathbf{r}', \mathcal{Z}) = 4iq \sum_{n=1}^{\infty} \sum_{\ell=0}^{n-1} \frac{2\ell+1}{4\pi} P_\ell(\mathbf{r}, \mathbf{r}') \frac{(n-\ell-1)!}{(n+\ell)!} \frac{1}{n+i\eta} e^{iq(r+r')} (-2iqr)^\ell (-2iqr')^\ell \\ \times L_{n-\ell-1}^{2\ell+1}(-2iqr) L_{n-\ell-1}^{2\ell+1}(-2iqr') \quad (37)$$

where  $L_n^\ell(x)$  is the Laguerre polynomial and  $q = (2\mathcal{Z})^{1/2}$ . Thus

$$I = 2(-2iq)^3 \left( \frac{d^2 A}{dp_1 dp_2} \right)_{p_1=p_2=\beta-iq} \quad (38)$$

where

$$A = \sum_{n=0}^{\infty} \frac{1}{n+2+i\eta} f_n(p_1) f_n(p_2) \frac{n!}{(n+3)^3} \quad (39)$$

and

$$f_n(p) = \int_0^\infty dr e^{-pr} r^3 L_n^3(-2iqr) = \frac{(n+3)!}{n!} \frac{x^n}{p^4} \quad (40)$$

with

$$\left( x = \frac{p+2iq}{p} \right). \quad (41)$$

Using the formula

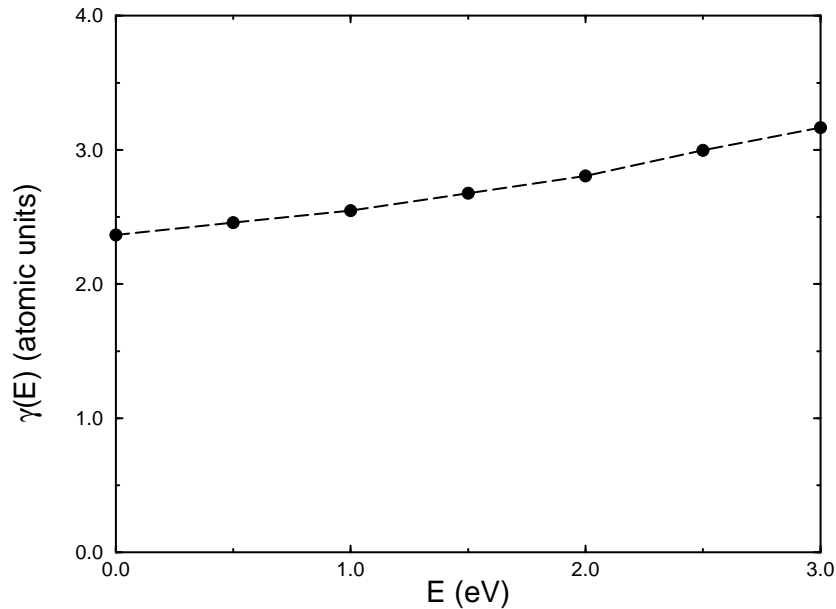
$$\sum_{n=0}^{\infty} \frac{1}{n+v} x^n = \frac{1}{v} {}_2F_1(1, v; v+1; x) \quad (42)$$

we obtain

$$A = \frac{1}{2+i\eta} \frac{1}{p_1^4 p_2^4} \frac{d^3}{dx^3} x^3 {}_2F_1(1, 2+i\eta; 3+i\eta; x) \quad (43)$$

where  $x = x_1 x_2$ . This yields

$$A = \frac{1}{2+i\eta} \frac{6}{p_1^4 p_2^4} {}_2F_1(4, 2+i\eta; 3+\eta; x). \quad (44)$$



**Figure 1.** The dependence on energy of the hydrogen atom polarization constant in atomic units.

Substituting this expression for  $A$  into equation (38) we obtain the ion-on-hydrogen atom polarization potential constant

$$\gamma = \frac{2^7 i q^3 Q^2}{2 + i\eta} \left[ \frac{16}{p^{10}} {}_2F_1(2 + i\eta, 4; 3 + i\eta; x) + \left( \frac{4}{p^{12}} c^2 - \frac{32}{p^{12}} (p - c)c \right) \frac{2 + i\eta}{3 + i\eta} {}_2F_1(3 + i\eta, 5; 4 + i\eta; x) + \frac{1}{p^{14}} (p - c)^2 c^2 \frac{20(2 + i\eta)}{4 + i\eta} {}_2F_1(4 + i\eta, 6; 5 + i\eta; x) \right] \quad (45)$$

with  $\eta = -\frac{i}{q}$ ,  $p = 1 - iq$ ,  $x = \frac{1+iq}{1-iq}$ ,  $c = -2iq$ .

Since  $q = (2E^c - 1)^{1/2}$  where  $E^c$  is the relative collision energy, the low-energy limit yields  $q \cong i$  and  $x \cong 0$  and hence  $\gamma \cong \frac{9}{4} Q^2$ , what is to be expected [2] from the known polarizability of atomic hydrogen. To illustrate the energy dependence of the polarization constant when the collision energy rises from zero we calculate  $\gamma$  in the energy range  $0 \leq E^c < 3$  eV. Our result is shown in figure 1 showing a relative change of  $\gamma$  of about 30%.

We also derive the representation for the hydrogen atom-ion polarization potential at asymptotically large distances,  $\rho \gg 1$ , which can be written in the form

$$V(\rho) = - \sum_{\ell=1}^{\infty} \frac{\gamma_{\ell}}{\rho^{2\ell+2}} \quad (46)$$

where

$$\gamma_{\ell} = \frac{8}{2\ell + 1} (-2iq)^{2\ell+1} Q^2 \left( \frac{d^2 A_{\ell}}{dp_1 dp_2} \right)_{p_1=p_2=1-iq} \quad (47)$$



and

$$A_\ell = \frac{(2\ell + 1)!}{\ell + 1 + i\eta} \frac{1}{(p_1 p_2)^{2\ell+2}} {}_2F_1(2\ell + 2, \ell + 1 + i\eta; \ell + 2 + i\eta; x_1 x_2). \quad (48)$$

We note that this result does not coincide with the well known expansion of polarization potential in [1]. The latter concerns high energies while our result is derived for low energies and is valid in the limit the  $k \rightarrow 0$ .

### 3.3. Ion–atom and atom–atom scattering

As a third example we investigate the properties of the polarization potential at high energy for ion–arbitrary atom and atom–atom scattering. Using the expression in equation (12) for the effective ion–atom or atom–atom potential

$$V_{\text{eff}} = V_{\text{st}} + V_{\text{pol}} \quad (49)$$

where  $V_{\text{st}}$  is defined by equation (13) and the high-energy approximation for the polarization potential

$$V_{\text{pol}} \cong \langle \phi_\alpha | V^\alpha \hat{G}_\alpha V^\alpha | \phi_\alpha \rangle \quad (50)$$

we obtain the representation of the elastic amplitude in the two-potential approximation form [9]:

$$t_{\text{el}}(\mathbf{p}, \mathbf{p}_0) = t_{\text{st}}(\mathbf{p}, \mathbf{p}_0) + \langle \mathbf{p}^{(-)} | V_{\text{pol}} | \mathbf{p}_0^{(+)} \rangle. \quad (51)$$

The amplitude  $t_{\text{st}}(\mathbf{p}, \mathbf{p}_0)$  in equation (51) corresponds to the scattering on the potential  $V_{\text{st}}$  while the states  $|\mathbf{p}^{(\pm)}\rangle$  are the distorted waves for this potential. At reasonably high energies we can use the eikonal approximation, which yields

$$\langle \mathbf{p} | \mathbf{p}^{(\pm)} \rangle = (2\pi)^{-3/2} \exp\left(i\mathbf{p}\boldsymbol{\rho} + \frac{\mu_\alpha}{ip} \int_{\mp\infty}^z dz' V_{\text{st}}(\mathbf{b}, z')\right) \quad (52)$$

and

$$t_{\text{st}}(\mathbf{p}, \mathbf{p}_0) = t_{\text{st}}(\mathbf{q}) = -\frac{ip}{(2\pi)^3 \mu_\alpha} \int d\mathbf{b} e^{iq\mathbf{b}} \left(1 - \exp\left(\frac{\mu_\alpha}{ip} \int_{-\infty}^{\infty} dz V_{\text{st}}(\mathbf{b}, z)\right)\right) \quad (53)$$

where  $\mathbf{q} = \mathbf{p}_0 - \mathbf{p}$  and  $\mathbf{b}$  are the momentum transfer and impact parameter, respectively.

Using the optical theorem and expanding the total reaction cross section as a power series in the parameter  $\frac{1}{v} = \frac{\mu_\alpha}{p_0}$  we find that the leading term of this power series has the form

$$\sigma_{\text{tot}} = \frac{\mu_\alpha^2}{p_0^2} \int d\mathbf{b} \left( \int d\mathbf{r} \int_{-\infty}^{\infty} dz |\phi_\alpha(\mathbf{r})|^2 V^\alpha(\mathbf{r}, \mathbf{b}) \right) - \frac{2(2\pi)^3 \mu_\alpha}{p_0} \text{Im} \langle \mathbf{p}_0 | V_{\text{pol}} | \mathbf{p}_0 \rangle. \quad (54)$$

In particular, the contribution of the Born terms of order higher than the second one are neglected in  $t_{\text{st}}(\mathbf{q})$ , leading to equation (54).

Next, the spectral representation of the Green function  $\hat{G}_\alpha(\mathcal{Z})$  is used to calculate the contribution of the polarization potential into equation (54)

$$\hat{G}_\alpha(\mathcal{Z}) = \sum_{i \neq 0} \frac{|\varphi_{\alpha i}\rangle \langle \varphi_{\alpha i}|}{\mathcal{Z} - \varepsilon_{\alpha i} - \frac{\hat{p}_\alpha^2}{2\mu_\alpha}} \quad (55)$$

where  $\{|\varphi_{\alpha i}\rangle\}$  is the complete set of target atom states,  $\varepsilon_{\alpha i}$  is the energy of the  $i$ th state,  $\varphi_{\alpha 0} = \phi_{\alpha}$  and  $\varepsilon_{\alpha 0} = -\kappa_{\alpha}^2$ , as well as the eikonal approximation for the matrix elements  $\langle \rho | (E + i0 - \varepsilon_{\alpha i} - \frac{\hat{p}_{\alpha}^2}{2\mu_{\alpha}})^{-1} | \rho' \rangle$ . As a result we find that

$$\sigma_{\text{tot}} = \frac{\mu_{\alpha}^2}{p_0} \sum_i \frac{1}{p_i} \phi_{\alpha}^*(\mathbf{r}) \varphi_{\alpha i}(\mathbf{r}) \phi_{\alpha}(\mathbf{r}') \varphi_{\alpha i}^*(\mathbf{r}') \times \int d\mathbf{b} \int_{-\infty}^{\infty} dz e^{-i\Delta_i z} V^{\alpha}(\mathbf{b}, z; \mathbf{r}) \cdot \int d\mathbf{b} \int_{-\infty}^{\infty} dz e^{-i\Delta_i z} V^{\alpha}(\mathbf{b}, z; \mathbf{r}') \quad (56)$$

where  $p_i = \sqrt{2\mu_{\alpha}(E - \varepsilon_{\alpha i})}$  and  $\Delta_i = p_0 - p_i$ .

Particularly in the case of ion-atom scattering, the potential  $V^{\alpha}$  has the form

$$V^{\alpha}(\mathbf{r}, \rho) = -Qe^2 \left( \sum_{i=1}^N \frac{1}{|\mathbf{r}_i - \rho|} - \frac{1}{\rho} \right) \quad (57)$$

where  $N$  is the number of electrons in the target atom. By using the integral representation of the McDonald function  $K_0(z)$

$$2K_0(z) = \int_{-\infty}^{\infty} dx \frac{e^{-ixz}}{\sqrt{1+x^2}} \quad (58)$$

and neglecting the difference between  $p_0$  and  $p_i$  in the denominators of equation (56) we obtain

$$\sigma_{\text{tot}} = \frac{4\mu_{\alpha}^2}{p_0^2} \sum_i \int d\mathbf{r} \int d\mathbf{r}' \phi_{\alpha}^*(\mathbf{r}) \varphi_{\alpha i}(\mathbf{r}) \phi_{\alpha}(\mathbf{r}') \varphi_{\alpha i}^*(\mathbf{r}') \int d\mathbf{b} \left( N^2 K_0^2(\Delta_i b) - N K_0(\Delta_i b) \times \left( \sum_{j=1}^N K_0(\Delta_i |\mathbf{b} - \mathbf{b}_j|) + \sum_{k=1}^N K_0(\Delta_i |\mathbf{b} - \mathbf{b}'_k|) \right) + \sum_{j=1}^N \sum_{k=1}^N K_0(\Delta_i |\mathbf{b} - \mathbf{b}_j|) K_0(\Delta_i |\mathbf{b} - \mathbf{b}'_k|) \right). \quad (59)$$

The limit  $\Delta_0 \rightarrow 0$  is implied in equation (59). To perform integration over the impact parameter  $\mathbf{b}$  we use the relations

$$\int d\mathbf{b} K_0^2(\Delta b) = \frac{\pi}{\Delta} \quad \int d\mathbf{b} K_0(\Delta b) K_0(\Delta |\mathbf{b} - \mathbf{b}_1|) = \frac{\pi}{\Delta} b_1 K_1(\Delta b_1). \quad (60)$$

From properties of the function  $K_1(z)$  of a small argument

$$K_1(z) \sim \frac{1}{z} + \frac{z}{2} \ln \frac{z}{2} - \frac{z}{4} (\psi(2) + \psi(1)) \quad z \rightarrow 0$$

where  $\psi(z)$  is the  $\psi$ -function, we obtain

$$\sigma_{\text{tot}} = \frac{4\pi Q^2}{v^2} (a \ln 2v + b) \quad (61)$$

where the constants  $a$  and  $b$  are defined by relations:

$$\begin{aligned}
 a &= N \int d\mathbf{b} \rho(\mathbf{b}) b^2 - N(N-1) \int d\mathbf{b}_1 \int d\mathbf{b}_2 f(\mathbf{b}_1, \mathbf{b}_2) \mathbf{b}_1 \mathbf{b}_2 \\
 b &= \frac{1}{2} N^2 (\psi(2) + \psi(1)) \int d\mathbf{b} \rho(\mathbf{b}) b^2 - N \int d\mathbf{b} \rho(\mathbf{b}) b^2 \ln b \\
 &\quad - \frac{1}{2} N(N-1) \int d\mathbf{b}_1 \int d\mathbf{b}_2 f(\mathbf{b}_1, \mathbf{b}_2) |\mathbf{b}_1 - \mathbf{b}_2|^2 \ln |\mathbf{b}_1 - \mathbf{b}_2| \\
 &\quad + N^2 \sum_{i \neq 0} \ln \varepsilon_{\alpha i} \int d\mathbf{b}_1 \int d\mathbf{b}_2 \rho_{0i}(\mathbf{b}_1) \rho_{0i}^*(\mathbf{b}_2) |\mathbf{b}_1 - \mathbf{b}_2|^2
 \end{aligned} \tag{62}$$

and

$$\begin{aligned}
 \rho(\mathbf{b}_1) &= \int_{-\infty}^{\infty} dz_1 \int d\mathbf{r}_2 \dots \int d\mathbf{r}_N |\phi_{\alpha}(\mathbf{r}_1, \dots, \mathbf{r}_N)|^2 \\
 f(\mathbf{b}_1, \mathbf{b}_2) &= \int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2 \int d\mathbf{r}_3 \dots \int d\mathbf{r}_N |\phi_{\alpha}(\mathbf{r}_1, \dots, \mathbf{r}_N)|^2 \\
 \rho_{0i}(\mathbf{b}_1) &= \int_{-\infty}^{\infty} dz_1 \int d\mathbf{r}_2 \dots \int d\mathbf{r}_N \phi_{\alpha}^*(\mathbf{r}_1, \dots, \mathbf{r}_N) \phi_{\alpha i}(\mathbf{r}_1, \dots, \mathbf{r}_N).
 \end{aligned} \tag{63}$$

The constant  $a$  determines the dipole momentum of the target atom

$$a = \langle \phi_{\alpha} | \left( \sum_{j=1}^N \mathbf{b}_j \right)^2 | \phi_{\alpha} \rangle = \langle \phi_{\alpha} | \mathbf{d}_{\perp}^2 | \phi_{\alpha} \rangle \tag{64}$$

where  $\mathbf{d}_{\perp}$  is the target dipole momentum projection onto the plane perpendicular to the vector  $\mathbf{p}_0$ . The constant  $b$  accounts for the dipole and quadrupole transitions in the target atom.

In the special case of the hydrogen atom these yield

$$\sigma_{\text{tot}} = \frac{8\pi}{v^2} \left( \ln 2v + \frac{3}{4} + \ln \frac{1}{\Delta E} \right) \tag{65}$$

where

$$\begin{aligned}
 \ln \frac{1}{\Delta E} &= \sum_{i \neq 0} S_i \ln \varepsilon_{\alpha i} \\
 S_i &= \int d\mathbf{b}_1 \int d\mathbf{b}_2 \rho_{0i}(\mathbf{b}_1) \rho_{0i}^*(\mathbf{b}_2) |\mathbf{b}_1 - \mathbf{b}_2|^2.
 \end{aligned} \tag{66}$$

It is interesting to note that the result in equation (61) can be also obtained by using the following approximation for the Green function  $\hat{G}_{\alpha}(\mathcal{Z})$  in equation (55) [1]

$$\hat{G}_{\alpha}(\mathcal{Z}) = \left( \mathcal{Z} - \tilde{\varepsilon} - \frac{\hat{p}_{\alpha}^2}{2\mu_{\alpha}} \right)^{-1} (I - |\phi_{\alpha}\rangle\langle\phi_{\alpha}|) \tag{67}$$

where the value  $\tilde{\varepsilon}$  is the average excitation energy of the atom. This yields

$$\sigma_{\text{tot}} = \frac{4\pi Q^2}{v^2} \left( a \ln \frac{1}{\Delta} + b' \right) \tag{68}$$

where  $\Delta = p_0 - \sqrt{p_0^2 - 2\mu_\alpha(\kappa^2 + \tilde{\epsilon})}$ , the value  $a$  has the same meaning as in the formula (61) and  $b'$  is obtained in the form

$$b' = N^2 \int d\mathbf{b} \rho(\mathbf{b}) b^2 \left( \frac{1}{2} + \psi(1) - \ln \frac{b}{2} \right) - \frac{1}{2} N(N-1) \int d\mathbf{b}_1 \times \int d\mathbf{b}_2 f(\mathbf{b}_1, \mathbf{b}_2) \left( \frac{1}{2} + \psi(1) - \ln \frac{|\mathbf{b}_1 - \mathbf{b}_2|}{2} \right). \quad (69)$$

This result for  $\sigma_{\text{tot}}$  is a justification of the approximation for the Green function in equation (67) as well as a direct method for calculation of the average excitation energy  $\tilde{\epsilon}$ .

### 3.4. Alternate derivation of scattering wavefunction

As our final example, we derive an expression for the scattering wavefunction  $|\Psi_\alpha^{(+)}\rangle$  which satisfies boundary conditions as given by the Lippmann–Schwinger equation

$$|\Psi_\alpha^{(+)}\rangle = |\phi_\alpha \mathbf{p}_0\rangle + \hat{G}_\alpha(E + i0) V^\alpha |\Psi_\alpha^{(+)}\rangle. \quad (70)$$

Approximation of the channel Green function in the form equation (67) yields for the solution of equation (70)

$$\langle \mathbf{r} \rho | \Psi_\alpha^{(+)}(\mathbf{p}_0) \rangle = (2\pi)^{-3/2} e^{ip_0 \rho} \phi_\alpha(\mathbf{r}) F(\mathbf{r}, \rho). \quad (71)$$

Therefore the function  $F(\mathbf{r}, \rho)$  satisfies the integral equation

$$F(\mathbf{r}, \rho) = 1 - \frac{\mu_\alpha}{2\pi} \int d\rho' \frac{e^{ip_0(z-z') + ip|\rho-\rho'|}}{|\rho-\rho'|} V^\alpha(\mathbf{r}, \rho') F(\mathbf{r}, \rho') \quad (72)$$

with  $p = p_0 - \Delta = \sqrt{p_0^2 - 2\mu_\alpha(\kappa^2 + \tilde{\epsilon})}$ . The  $z$ -axis is chosen parallel to the vector  $\mathbf{p}_0$ . The kernel of equation (72) contains the large parameter  $p$ , so that we can apply asymptotic methods to construct the solution of this equation. Application of the stationary phase method results in the equation

$$F(z) = 1 + \frac{\mu_\alpha}{ip} \int_{-\infty}^{\infty} dz' e^{ip_0(z'-z) + ip|z-z'|} V^\alpha(z') F(z') \quad (73)$$

where, for simplicity, we omit dependence on all variables with the exception of the  $z$  coordinate. Neglecting the terms of orders higher than  $p^{-1}$ , this reduces to the expression

$$F(z) = 1 + \frac{\mu_\alpha}{ip} \int_{-\infty}^z dz' e^{-i\Delta(z-z')} V^\alpha(z') F(z') \quad (74)$$

which can be transformed into

$$F(z) = 1 + \frac{\mu_\alpha}{ip} \int_{-\infty}^z dz' e^{-i\Delta(z-z')} V^\alpha(z') e^{\frac{\mu_\alpha}{ip} \int_{z'}^z dz'' V^\alpha(z'')}. \quad (75)$$

This yields the elastic scattering amplitude in the form

$$t_{\text{el}}(\mathbf{p}, \mathbf{p}_0) = \langle \mathbf{p} \phi_\alpha | V^\alpha | \Psi_\alpha^{(+)}(\mathbf{p}_0) \rangle = \frac{1}{(2\pi)^3} \int d\rho e^{iq\rho} \int d\mathbf{r} |\phi_\alpha(\mathbf{r})|^2 V^\alpha(\mathbf{r}, \rho) + \frac{\mu_\alpha}{ip} \frac{1}{(2\pi)^3} \int d\mathbf{r} |\phi_\alpha(\mathbf{r})|^2 \int d\mathbf{b} \int_{-\infty}^{\infty} dz \int_{-\infty}^z dz' V^\alpha(\mathbf{r}; \mathbf{b}, z) V^\alpha(\mathbf{r}; \mathbf{b}, z') \times e^{-i\Delta(z-z')} e^{\frac{\mu_\alpha}{ip} \int_{z'}^z dz'' V^\alpha(\mathbf{r}; \mathbf{b}, z'')}. \quad (76)$$

At high energy, the representation given by equation (76) leads to the same result for the reaction total cross section as that derived from the polarization potential approach.

Therefore the representation in equations (71) and (75) of the scattering wavefunction properly takes into account the effect of the polarization potential in distinction to the traditional eikonal approximation, which can be obtained from (75) by neglecting the value  $\Delta$ . This fact explains why the elastic amplitude written within the framework of the traditional eikonal approximation diverges in the forward direction [18].

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