Long-range behavior of the optical potential for the elastic scattering of charged composite particles

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Abstract

The asymptotic behavior of the optical potential, describing elastic scattering of a charged particle α off a bound state of two charged, or one charged and one neutral, particles at small momentum transfer Δ_{α} or equivalently at large intercluster distance ρ_{α} , is investigated within the framework of the exact three-body theory. For the three-charged-particle Green function that occurs in the exact expression for the optical potential, a recently derived expression, which is appropriate for the asymptotic region under consideration, is used. We find that for arbitrary values of the energy parameter the non-static part of the optical potential behaves for $\Delta_{\alpha} \to 0$ as $C_1\Delta_{\alpha} + o(\Delta_{\alpha})$. From this we derive for the Fourier transform of its onshell restriction for $\rho_{\alpha} \to \infty$ the behavior $-a/2\rho_{\alpha}^4 + o(1/\rho_{\alpha}^4)$, i.e., dipole or quadrupole terms do not occur in the coordinate-space asymptotics. This result corroborates the standard one, which is obtained by perturbative methods. The general, energy-dependent expression for the dynamic polarisability C_1 is derived; on the energy shell it reduces to the conventional polarisability a which is independent of the energy. We emphasize that the present derivation is *non-perturbative*, i.e., it does not make use of adiabatic or similar approximations, and is valid for energies below as well as above the three-body dissociation threshold. 03.65.Nk, 34.40.+n, 24.10.-i, 21.45.+v

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I. INTRODUCTION

The incorporation of the long-ranged Coulomb interaction in the theoretical description of reactions between charged composite particles constitutes a problem of longstanding interest, due to its great importance in atomic and nuclear physics. As a prototype we consider the elastic scattering of a charged particle off a cluster composed of two charged (or one charged and one neutral) particles.

Formally, such a reaction can be described in terms of a single-channel Lippmann-Schwinger-type integral equation for the elastic scattering amplitude, in which the socalled optical potential occurs (see, e.g., [1,2]). Although the latter is structurally too complicated for practical purposes (besides being non-local, energy-dependent, and complex above the threshold for the opening of the lowest inelastic channel, it contains the three-body Green function which is actually the object whose calculation is attempted), its very existence is of considerable significance for many purposes.

An alternative formulation is based on the exact three-particle equations [3], suitably generalized to accommodate the long-ranged Coulomb potentials either in coordinate [4], or in momentum space [5–9]. The latter approach leads to coupled multichannel Lippmann-Schwinger-type equations whose solution yield simultaneously all twofragment, i.e. the (in-)elastic and rearrangement, amplitudes (and with an additional quadrature also the dissociation amplitudes). For three charged particles, the effective potentials occurring therein are again too complicated to be used presently for practical calculations (except with drastic approximations). But, if only two of the three particles are charged, some version [7] of these equations becomes manageable, and has in fact already been applied successfully to the calculation of elastic scattering and breakup observables in the proton-deuteron system [10,11].

Due to the differences in the physical pictures on which these two formulations are based, the expressions for the optical potential and for the effective potential as used in conventional applications of the three-body theory, differ appreciably (indeed, in ref. [12] it has been shown that the former can be derived within the framework of the threebody theory only under very special and unusual assumptions). It is therefore of general interest to gain insight into such properties of effective potentials, which do not depend on the specific details of the formulation, and are therefore common to both of them. One important example is the behavior for large separation of the colliding particles which should be similar in both cases, in contrast to the short-range behavior which in general will be rather different.

In the present investigation we concentrate on the optical potential. It is known to simplify considerably when the distance between the colliding particles goes to infinity, or equivalently when the momentum transfer goes to zero. In fact, its large-distance behavior has been extracted long time ago by various perturbative methods below [13,14], and recently also above [15] (cf. also [16,17]) the dissociation threshold. The result is wellknown: besides the static potential which comprises the multipole contributions arising from the charge distribution of the composite particle, the first non-vanishing term of longest range is the (local) polarisation potential (proportional to the inverse fourth power of the distance between the two colliding bodies). But in none of these investigations the reliability of the approximate, or the convergence of the perturbative, treatment has been studied.

However, precise knowledge of the asymptotic behavior of the optical potential is of great interest, for many reasons: not only does it constrain the construction of (the longrange part of) model optical potentials for practical applications; but it also provides answers to crucial questions like, e.g., what kind of effective-range expansion be adequate or what rate of convergence of partial-wave sums is to be expected.

For these reasons, there have recently appeared several attempts to provide nonperturbative derivations based on three-body theory, both in coordinate [18] and in momentum [19–23] space. Indeed, it was found that the above mentioned, approximately derived long-range behavior could be recovered. However, not only are these investigations lacking the rigour, and often also the generality, desirable in view of the significance of the result. What is much more restrictive is that these proofs could be established only for energies *below the three-body dissociation threshold*.

In the present paper we give, based on the three-body integral equations approach in momentum space, a *non-perturbative* derivation of the behavior of the optical potential as the momentum transfer goes to zero, which is valid *both below and above* the threebody dissociation threshold, and which does not suffer from the shortcomings of the previous attempts. Of course, this momentum-transfer behavior determines the largedistance behavior in coordinate space. At the same time we deduce the general (energydependent) form of the induced dipole polarisability. For this purpose, use is made of the recently developed asymptotic form of the wave function for three charged particles in the continuum or equivalently of the asymptotic expression for the three-charged-particle Green function [24], that applies to just that region of the three-body configuration space which is relevant in the present context.

The paper is organized as follows. In Sec. II we briefly recapitulate the formulation of the optical potential for elastic scattering from the *m*-th bound state (either ground or excited state) of the composite particle within the framework of the three-body theory. When writing down explicitly its leading term in the limit of vanishing momentum transfer, the above mentioned asymptotic expression for the three-charged-particle Green function is introduced. The behavior of the optical potential as the momentum transfer goes to zero is derived in Sec. III. There we also present the general expression of the induced dipole polarisability. These results are then specialized to on-shell scattering, both in momentum and in coordinate space. The Summary contains a discussion of our achievements. Several auxiliary results are collected in the Appendices.

We mention that throughout we use natural units, i.e., $\hbar = c = 1$. Furthermore, unit vectors will be denoted by a hat, i. e., $\hat{a} \equiv \mathbf{a}/a$.

II. THE OPTICAL POTENTIAL

A. Definition of the optical potential

Consider three distinguishable particles with masses m_{ν} and charges e_{ν} , $\nu = 1, 2, 3$. We use Jacobi coordinates: $\mathbf{p}_{\alpha} (\mathbf{r}_{\alpha})$ is the relative momentum (coordinate) between particles β and γ , and $\mu_{\alpha} = m_{\beta}m_{\gamma}/(m_{\beta} + m_{\gamma})$ their reduced mass; $\mathbf{q}_{\alpha} (\boldsymbol{\rho}_{\alpha})$ denotes the relative momentum (coordinate) between particle α and the center of mass of the pair $(\beta\gamma)$, the corresponding reduced mass being defined as $M_{\alpha} = m_{\alpha}(m_{\beta} + m_{\gamma})/(m_{\alpha} + m_{\beta} + m_{\gamma})$.

The Hamiltonian of the three-body system is

$$H = H_0 + V = H_0 + \sum_{\nu=1}^3 V_{\nu}, \tag{1}$$

with H_0 being the free three-body Hamiltonian, and

$$V_{\alpha} = V_{\alpha}^{S} + V_{\alpha}^{C} \tag{2}$$

the full interaction between particles β and γ , consisting of a short-range (V_{α}^{S}) and a Coulombic part,

$$V_{\alpha}^{C}(\mathbf{r}_{\alpha}) = \frac{e_{\beta}e_{\gamma}}{r_{\alpha}}.$$
(3)

The three-body transition operator $U_{\alpha\alpha}(z)$ which describes elastic and inelastic scattering in channel α , satisfies the equation

$$U_{\alpha\alpha}(z) = \bar{V}_{\alpha} + \bar{V}_{\alpha}G_{\alpha}(z)U_{\alpha\alpha}(z).$$
(4)

Herein,

$$\bar{V}_{\alpha} = \sum_{\nu} \bar{\delta}_{\nu\alpha} V_{\nu} = \bar{V}_{\alpha}^{S} + \bar{V}_{\alpha}^{C} = \sum_{\nu} \bar{\delta}_{\nu\alpha} V_{\nu}^{S} + \sum_{\nu} \bar{\delta}_{\nu\alpha} V_{\nu}^{C}$$
(5)

is the channel interaction and

$$G_{\alpha}(z) = (z - H_{\alpha})^{-1} = (z - H_0 - V_{\alpha})^{-1}$$
(6)

the channel Green function. The conventional notation $\bar{\delta}_{\nu\alpha} = 1 - \delta_{\nu\alpha}$ for the anti-Kronecker symbol has been used. Let $|\psi_{\alpha m}\rangle$ be the (normalized) bound state wave function (belonging to the binding energy $\hat{E}_{\alpha m}$, which we assume to be non-degenerate) of the pair $(\beta \gamma)_m$, where the index m denotes the complete set of quantum numbers. The notation is to indicate that we allow the pair to be either in the ground or in some excited state. The free motion of particle α relative to the center of mass of $(\beta \gamma)_m$ is described by the plane wave $|\mathbf{q}_{\alpha}\rangle$. Then the quantity

$$\mathcal{T}_{\alpha m,\alpha m}(\mathbf{q}'_{\alpha},\mathbf{q}_{\alpha};E) = \langle \mathbf{q}'_{\alpha} | \mathcal{T}_{\alpha m,\alpha m}(E+i0) | \mathbf{q}_{\alpha} \rangle, \tag{7}$$

with

$$\mathcal{T}_{\alpha m,\alpha m}(z) = \langle \psi_{\alpha m} | U_{\alpha \alpha}(z) | \psi_{\alpha m} \rangle, \tag{8}$$

is on the energy shell, i.e., for

$$E = E_{\alpha m} \equiv \bar{q}_{\alpha}^2 / 2M_{\alpha} + \hat{E}_{\alpha m}, \quad q_{\alpha}' = q_{\alpha} = \bar{q}_{\alpha}, \tag{9}$$

the physical amplitude amplitude for elastic scattering of particle α off the bound state $(\beta \gamma)_m$.

Equation (4) by itself does not yet lead to the desired Lippmann-Schwinger (LS)-type equation for the effective-two-body elastic scattering operator $\mathcal{T}_{\alpha m,\alpha m}(z)$ since the spectral decomposition of $G_{\alpha}(z)$ contains contributions not only from the *m*-th but also from all the other bound states, and in particular also from the continuum states, in subsystem α . This goal is achieved, e.g., by means of the Feshbach projection operator technique [25]. Introduce the projector onto the target state and its orthogonal complement,

$$P_{\alpha m} = |\psi_{\alpha m}\rangle\langle\psi_{\alpha m}|, \qquad Q_{\alpha m} = 1 - P_{\alpha m}.$$
(10)

Then

$$G_{\alpha}(z) = P_{\alpha m} G_{\alpha}(z) + Q_{\alpha m} G_{\alpha}(z)$$

= $G_{\alpha}^{P}(z) + G_{\alpha}^{Q}(z),$ (11)

with

$$\langle \mathbf{q}_{\alpha}' | G_{\alpha}^{P}(z) | \mathbf{q}_{\alpha} \rangle = | \psi_{\alpha m} \rangle \frac{\delta(\mathbf{q}_{\alpha}' - \mathbf{q}_{\alpha})}{z - q_{\alpha}^{2}/2M_{\alpha} - \hat{E}_{\alpha m}} \langle \psi_{\alpha m} |, \qquad (12)$$

represents a splitting of the channel Green function into a term (12) which is separable (with respect to the variables internal to subsystem α), and a remainder. Introducing the decomposition (11) in (4) yields, e.g. through application of the AGS reduction procedure [26],

$$\mathcal{T}_{\alpha m,\alpha m}(z) = \mathcal{V}_{\alpha m,\alpha m}^{opt}(z) + \mathcal{V}_{\alpha m,\alpha m}^{opt}(z) \frac{1}{z - \mathbf{Q}_{\alpha}^2/2M_{\alpha} + \hat{E}_{\alpha m}} \mathcal{T}_{\alpha m,\alpha m}(z).$$
(13)

For convenience we have introduced the relative momentum operator \mathbf{Q}_{α} whose eigenvalue is \mathbf{q}_{α} . Equation (13) is the desired one-channel operator LS equation for the elastic scattering amplitude. The plane wave matrix elements of potential operator

$$\mathcal{V}_{\alpha m,\alpha m}^{opt}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};z) = \langle \mathbf{q}_{\alpha}' | \langle \psi_{\alpha m} | \bar{V}_{\alpha} + \bar{V}_{\alpha} Q_{\alpha m} \frac{1}{z - H_{\alpha} - Q_{\alpha m} \bar{V}_{\alpha} Q_{\alpha m}} Q_{\alpha m} \bar{V}_{\alpha} | \psi_{\alpha m} \rangle | \mathbf{q}_{\alpha} \rangle$$
$$= \langle \mathbf{q}_{\alpha}' | \langle \psi_{\alpha m} | \bar{V}_{\alpha} + \bar{V}_{\alpha} G^{Q}(z) \bar{V}_{\alpha} | \psi_{\alpha m} \rangle | \mathbf{q}_{\alpha} \rangle \tag{14}$$

are seen to coincide with the standard definition of the optical potential. Here, the identity

$$Q_{\alpha m}[z - H_{\alpha} - Q_{\alpha m}\bar{V}_{\alpha}Q_{\alpha m}]^{-1}Q_{\alpha m} = Q_{\alpha m}G(z)Q_{\alpha m} =: G^{Q}(z),$$
(15)

 $G(z) = (z-H)^{-1}$ being the resolvent of the full Hamiltonian H, has been used. Of course, this expression for the optical potential can also be derived directly from the Schrödinger equation. Its relation to the effective potentials introduced in the three-body theory has been described in [12].

The question of the solvability of an equation like (13) depends crucially on the singular behavior of the effective potential $\mathcal{V}_{\alpha m,\alpha m}^{opt}(\mathbf{q}'_{\alpha},\mathbf{q}_{\alpha};E)$ in the limit that the momentum transfer

$$\Delta_{\alpha} = \mathbf{q}_{\alpha}' - \mathbf{q}_{\alpha} \tag{16}$$

goes to zero. In leading order the latter is defined entirely by the Coulombic part \bar{V}^{C}_{α} of the channel interaction, i.e., it does depend neither on the short-ranged part \bar{V}^{S}_{α} nor on the internal interaction V_{α} . Of course, a given behavior of the optical potential for $\Delta_{\alpha} \to 0$ reflects itself in a corresponding asymptotic behavior in coordinate space.

B. Explicit expression

In this section we establish the explicit expression of the optical potential which will be used in the following investigation of its analytical behavior in the limit $\Delta_{\alpha} \to 0$.

Let us rewrite (14) as

$$\mathcal{V}_{\alpha m,\alpha m}^{opt}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) = \mathcal{V}_{\alpha m,\alpha m}^{opt\,(1)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha}) + \mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E),\tag{17}$$

with

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(1)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha}) = \langle \mathbf{q}_{\alpha}' | \langle \psi_{\alpha m} | \bar{V}_{\alpha} | \psi_{\alpha m} \rangle | \mathbf{q}_{\alpha} \rangle, \tag{18}$$

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) = \langle \mathbf{q}_{\alpha}' | \langle \psi_{\alpha m} | \bar{V}_{\alpha} G^Q(E+i0) \bar{V}_{\alpha} | \psi_{\alpha m} \rangle | \mathbf{q}_{\alpha} \rangle. \tag{19}$$

The first term (18) on the r.h.s. of (17), which is called the static potential, has for $\Delta_{\alpha} \to 0$ only the trivial Coulomb-type singular behavior

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(1)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha}) \stackrel{\Delta_{\alpha}\to0}{\approx} \langle \mathbf{q}_{\alpha}' | \langle \psi_{\alpha m} | \bar{V}_{\alpha}^{C} | \psi_{\alpha m} \rangle | \mathbf{q}_{\alpha} \rangle$$
$$\stackrel{\Delta_{\alpha}\to0}{=} \frac{4\pi e_{\alpha}(e_{\beta}+e_{\gamma})}{\Delta_{\alpha}^{2}} + \cdots$$
(20)

(the dots are to indicate terms $\sim \Delta_{\alpha}^{-1}$ and $\sim \ln \Delta_{\alpha}$ which may arise, e.g., if the target state is not spherically symmetric). It can be taken care of in the LS equation (13) in the usual manner (see, e.g., [9]).

Consequently the decisive question concerns the behavior of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\mathbf{q}'_{\alpha},\mathbf{q}_{\alpha};E)$ in the limit of zero momentum transfer. In lowest order perturbation theory, which in the present language is equivalent to approximating in (19) the full three-body Green function G(z) by its lowest order approximation $G_{\alpha}(z)$, and by taking into account that only the Coulombic part \bar{V}_{α}^{C} of the channel potential contributes to the leading singular behavior, one has on the energy shell the well-known result

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E_{\alpha m}) \stackrel{\Delta_{\alpha}\to 0}{\approx} \langle \mathbf{q}_{\alpha}' | \langle \psi_{\alpha m} | \bar{V}_{\alpha}^{C} G_{\alpha}^{Q}(E_{\alpha m}+i0) \bar{V}_{\alpha}^{C} | \psi_{\alpha m} \rangle | \mathbf{q}_{\alpha} \rangle \stackrel{\Delta_{\alpha}\to 0}{\sim} \Delta_{\alpha}, \qquad (21)$$

or in coordinate space

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\boldsymbol{\rho}_{\alpha}) \stackrel{\rho_{\alpha} \to \infty}{\approx} -\frac{a}{2\rho_{\alpha}^{4}},\tag{22}$$

for all energies. The factor *a* represents the polarizability of the composite particle. However, it is of outstanding importance to know whether this fundamental result holds also for the exact optical potential (19), i.e., even after all terms of the perturbation expansion of G(z) are summed up. In fact, for energies below the three-body dissociation threshold, i.e. for E < 0, it has been suggested in [18–23] that (21) remains true also for the exact expression (19). It is the purpose of the present investigation to derive its behavior for arbitrary E, that is in particular also for E > 0.

Let us write down the matrix element (19) explicitly in the coordinate-space representation,

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) = \sum_{\nu} \bar{\delta}_{\nu\alpha} \sum_{\mu} \bar{\delta}_{\mu\alpha} \int d\boldsymbol{\rho}_{\alpha}' d\mathbf{r}_{\alpha}' d\boldsymbol{\rho}_{\alpha} d\mathbf{r}_{\alpha} e^{-i\mathbf{q}_{\alpha}'\cdot\boldsymbol{\rho}_{\alpha}'} \\ \times \psi_{\alpha m}^{*}(\mathbf{r}_{\alpha}') V_{\mu}(\epsilon_{\alpha\mu}\boldsymbol{\rho}_{\alpha}' - \lambda_{\mu}\mathbf{r}_{\alpha}') G^{Q}(\boldsymbol{\rho}_{\alpha}',\mathbf{r}_{\alpha}';\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha};E+i0) \\ \times V_{\nu}(\epsilon_{\alpha\nu}\boldsymbol{\rho}_{\alpha} - \lambda_{\nu}\mathbf{r}_{\alpha}) \psi_{\alpha m}(\mathbf{r}_{\alpha}) e^{-i\mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}}.$$
(23)

For convenience, we have introduced the antisymmetric symbol $\epsilon_{\beta\alpha} = -\epsilon_{\alpha\beta}$, with $\epsilon_{\alpha\beta} = +1$ for (α, β) being a cyclic ordering of (1, 2, 3), and the mass ratios $\lambda_{\nu} = m_{\nu}/(m_{\beta} + m_{\gamma})$, for $\nu = \beta, \gamma$.

To further evaluate expression (23), the spectral decomposition of the kernel of $G^Q(E+i0)$ must be inserted and then the integrations over \mathbf{r}_{α} , $\boldsymbol{\rho}_{\alpha}$, \mathbf{r}'_{α} and $\boldsymbol{\rho}'_{\alpha}$ must be carried out. This requires in principle the knowledge of all the solutions of the full three-body Schrödinger equation

$$\left\{ E - T_{\mathbf{r}_{\alpha}} - T\boldsymbol{\rho}_{\alpha} - \sum_{\nu=1}^{3} V_{\nu} \right\} \Psi^{(+)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = 0, \qquad (24)$$

whether they describe states with asymptotically two or three unbound particles. Only the states corresponding to the discrete spectrum of H, i.e. three-body bound states, are not needed since they do not contribute to a singular behavior of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}$ in this limit (the reason being simply that they yield only terms which are separable in the incoming and outgoing momenta and thus do not depend on the momentum transfer at all). Here, $T_{\mathbf{r}_{\alpha}}$ is the kinetic energy operator for the relative motion of particles β and γ , and $T_{\boldsymbol{\rho}_{\alpha}}$ the one for the motion of particle α relative to the center of mass of the pair $(\beta\gamma)_m$. They are defined as

$$T_{\mathbf{r}_{\alpha}} = -\frac{\Delta_{\mathbf{r}_{\alpha}}}{2\mu_{\alpha}}, \qquad T\boldsymbol{\rho}_{\alpha} = -\frac{\Delta\boldsymbol{\rho}_{\alpha}}{2M_{\alpha}}.$$
(25)

The solutions of (24) are not known, but also not really needed. For, we are interested only in the behavior of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}$ for $\Delta_{\alpha} \to 0$. Below it will be shown that in this limit the leading, Δ_{α} -dependent term is defined by the singularities resulting from the divergence of the integrals in (23) over $\boldsymbol{\rho}_{\alpha}$ for $\rho_{\alpha} \to \infty$, and over $\boldsymbol{\rho}'_{\alpha}$ for $\rho'_{\alpha} \to \infty$. (Compare the discussion for an analogous two-body problem in ref. [28]). The integrals over \mathbf{r}_{α} and \mathbf{r}'_{α} do not induce a singular behavior. For, the wave functions $\psi_{\alpha m}(\mathbf{r}_{\alpha})$ and $\psi^*_{\alpha m}(\mathbf{r}'_{\alpha})$ of the incoming and outgoing bound pair $(\beta\gamma)_m$, respectively, practically confine the region of integration over the magnitudes of the subsystem-internal variables \mathbf{r}_{α} and \mathbf{r}'_{α} to values $r_{\alpha}, r'_{\alpha} \leq \kappa_{\alpha m}^{-1}$, where $\kappa_{\alpha m} = \sqrt{2\mu_{\alpha}|\hat{E}_{\alpha m}|}$. For this reason, when investigating the behavior of the leading term of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}$ in the limit $\Delta_{\alpha} \to 0$ it suffices to know the Green function $G^Q(\boldsymbol{\rho}'_{\alpha}, \mathbf{r}'_{\alpha}; \boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha}; E + i0)$ in the asymptotic region

$$\Omega_{\alpha} \cap \Omega_{\alpha}^{\prime},\tag{26}$$

with

$$\Omega_{\alpha}: \quad r_{\alpha}/\rho_{\alpha} \to 0, \quad \rho_{\alpha} \to \infty, \tag{27}$$

$$\Omega'_{\alpha}: \quad r'_{\alpha}/\rho'_{\alpha} \to 0, \quad \rho'_{\alpha} \to \infty.$$
(28)

In Ω_{α} the Hamiltonian *H* takes the form

$$H \xrightarrow{\Omega_{\alpha}} H_{\alpha}^{as} = T_{\mathbf{r}_{\alpha}} + T_{\boldsymbol{\rho}_{\alpha}} + V_{\alpha}(\mathbf{r}_{\alpha}) + v_{\alpha}^{C}(\boldsymbol{\rho}_{\alpha}),$$
(29)

where

$$v_{\alpha}^{C}(\boldsymbol{\rho}_{\alpha}) = \lim_{\rho_{\alpha} \to \infty, r_{\alpha}/\rho_{\alpha} \to 0} \left\{ V_{\beta}(\epsilon_{\alpha\beta}\boldsymbol{\rho}_{\alpha} - \lambda_{\beta}\mathbf{r}_{\alpha}) + V_{\gamma}(\epsilon_{\alpha\gamma}\boldsymbol{\rho}_{\alpha} - \lambda_{\gamma}\mathbf{r}_{\alpha}) \right\} = \frac{e_{\alpha}\left(e_{\beta} + e_{\gamma}\right)}{\rho_{\alpha}} \quad (30)$$

is the Coulomb potential between the charge e_{α} of particle α and the total charge $(e_{\beta}+e_{\gamma})$ of the particles β and γ concentrated in their center of mass. Because of this property $v_{\alpha}^{C}(\boldsymbol{\rho}_{\alpha})$ is termed 'center-of-mass Coulomb potential for channel α '. Note that in the region Ω_{α} we could neglect in (30) the short-range interactions between particles α and γ , and α and β , completely, and terms $\sim r_{\alpha}/\rho_{\alpha}^{2}$ in the corresponding Coulombian parts. The well-known class of solutions of the asymptotic Schrödinger equation

$$\{E - H^{as}_{\alpha}\} \Psi^{(+)as}_{\mathbf{q}^{0}_{\alpha}m}(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha}) = 0, \qquad (31)$$

belonging to the three-body energy $E = q_{\alpha}^{0^2}/2M_{\alpha} + \hat{E}_{\alpha m}$, is given by

$$\Psi_{\mathbf{q}_{\alpha}^{0}m}^{(+)as}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha}) = \psi_{\alpha m}(\mathbf{r}_{\alpha})\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}).$$
(32)

They consist of a product of the bound state wave function of the pair $(\beta \gamma)_m$ introduced above, which satisfies the two-body Schrödinger equation (we use the same symbols for operators acting in the two- and in the three-particle space)

$$\left\{ \hat{E}_{\alpha m} - T_{\mathbf{r}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha}) \right\} \psi_{\alpha m}(\mathbf{r}_{\alpha}) = 0, \qquad (33)$$

and the 'center-of-mass Coulomb scattering wave function', satisfying

$$\left\{\frac{q_{\alpha}^{0^2}}{2M_{\alpha}} - T\boldsymbol{\rho}_{\alpha} - v_{\alpha}^C(\boldsymbol{\rho}_{\alpha})\right\} \psi_{\mathbf{q}_{\alpha}^0}^{(+)}(\boldsymbol{\rho}_{\alpha}) = 0.$$
(34)

The solution of (34) is explicitly known,

$$\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}) = e^{i\mathbf{q}_{\alpha}^{0}\cdot\boldsymbol{\rho}_{\alpha}}\bar{N}_{\alpha}^{0}F(-i\bar{\eta}_{\alpha}^{0},1;i(q_{\alpha}^{0}\boldsymbol{\rho}_{\alpha}-\mathbf{q}_{\alpha}^{0}\cdot\boldsymbol{\rho}_{\alpha})),\tag{35}$$

with

$$\bar{\eta}^0_{\alpha} = \frac{e_{\alpha}(e_{\beta} + e_{\gamma})M_{\alpha}}{q^0_{\alpha}}, \quad \bar{N}^0_{\alpha} = e^{-\pi\bar{\eta}^0_{\alpha}/2}\,\Gamma(1 + i\bar{\eta}^0_{\alpha}). \tag{36}$$

Here, $\Gamma(x)$ denotes the Gamma function, and F(a, b; x) the confluent hypergeometric function [27]. Note that eventual bound state solutions of (34) for an attractive centerof-mass Coulomb potential are of no interest in the present context since they would correspond to a situation with all three particles being confined (see below).

We also need the solution of the asymptotic Schrödinger equation (31) with all three particles asymptotically in the continuum, i.e., the one which belongs to the three-body energy $E = q_{\alpha}^{02}/2M_{\alpha} + k_{\alpha}^{02}/2\mu_{\alpha}$. It will be called asymptotic continuum solution of the Schrödinger equation in Ω_{α} . This solution has been found in [24], and has the form

$$\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha}) = \psi_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha}) e^{i\mathbf{q}_{\alpha}^{0}\cdot\boldsymbol{\rho}_{\alpha}} e^{i\eta_{\beta}^{0}ln(k_{\beta}^{0}\boldsymbol{\rho}_{\alpha}-\epsilon_{\alpha\beta}\mathbf{k}_{\beta}^{0}\cdot\boldsymbol{\rho}_{\alpha})} e^{i\eta_{\gamma}^{0}ln(k_{\gamma}^{0}\boldsymbol{\rho}_{\alpha}-\epsilon_{\alpha\gamma}\mathbf{k}_{\gamma}^{0}\cdot\boldsymbol{\rho}_{\alpha})}.$$
(37)

The Coulomb parameters are given as

$$\eta_{\beta}^{0} = \frac{e_{\alpha}e_{\gamma}\mu_{\beta}}{k_{\beta}^{0}}, \quad \eta_{\gamma}^{0} = \frac{e_{\alpha}e_{\beta}\mu_{\gamma}}{k_{\gamma}^{0}}, \tag{38}$$

and the momenta \mathbf{k}^0_{β} and \mathbf{k}^0_{γ} are defined as the usual linear combinations of \mathbf{k}^0_{α} and \mathbf{q}^0_{α} ,

$$\mathbf{k}_{\nu}^{0} = \epsilon_{\alpha\nu}\mu_{\alpha}\mathbf{q}_{\alpha}^{0}/M_{\nu} - \lambda_{\nu}\mathbf{k}_{\alpha}^{0}, \quad \text{with} \quad \nu = \beta, \gamma.$$
(39)

The wave function $\psi_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha})$ is the continuum solution of the two-body-like Schrödinger equation

$$\left\{\frac{k_{\alpha}^{0\,2}(\boldsymbol{\rho}_{\alpha})}{2\mu_{\alpha}} - T_{\mathbf{r}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha})\right\}\psi_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha}) = 0,$$
(40)

with

$$\mathbf{k}^{0}_{\alpha}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}^{0}_{\alpha} + \frac{\mathbf{a}_{\alpha}(\hat{\boldsymbol{\rho}}_{\alpha})}{\rho_{\alpha}},\tag{41}$$

$$\mathbf{a}_{\alpha}(\hat{\boldsymbol{\rho}}_{\alpha}) = -\sum_{\nu} \bar{\delta}_{\nu\alpha} \eta^{0}_{\nu} \lambda_{\nu} \frac{\epsilon_{\alpha\nu} \hat{\boldsymbol{\rho}}_{\alpha} - \mathbf{k}^{0}_{\nu}}{1 - \epsilon_{\alpha\nu} \hat{\boldsymbol{\rho}}_{\alpha} \cdot \hat{\mathbf{k}}^{0}_{\nu}},\tag{42}$$

describing the relative motion of particles β and γ with *local* energy $E_{\alpha}(\boldsymbol{\rho}_{\alpha}) = k_{\alpha}^{0\,2}(\boldsymbol{\rho}_{\alpha})/2\mu_{\alpha}$. Thus it is, in fact, a three-body wave function, the influence of the presence of the third particle α however being confined to a shift of the two-body relative momentum of particles β and γ from its asymptotic (for $\rho_{\alpha} \to \infty$, i.e. particle α is infinitely far apart) value \mathbf{k}_{α}^{0} to the *local* value $\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})$. The latter depends explicitly on the distance of particle α from the center of mass of the pair $(\beta\gamma)_{m}$ as a result of long-ranged three-body correlations. Nevertheless, it is to be noted that, since $\boldsymbol{\rho}_{\alpha}$ enters the Schrödinger equation (40) only parametrically via the local energy, its solutions $\psi_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})(\mathbf{r}_{\alpha})$ and the genuine two-body bound state wave functions $\psi_{\alpha m}(\mathbf{r}_{\alpha})$, which are solutions of (33), are eigenfunctions of the same Hamiltonian $\{T_{\mathbf{r}_{\alpha}} + V_{\alpha}(\mathbf{r}_{\alpha})\}$ to different eigenvalues, and are therefore orthogonal.

Let us add two comments.

1) It has to be pointed out that (37) is valid in all of Ω_{α} , except for the so-called singular directions which are defined by the conditions $\epsilon_{\alpha\beta}\hat{\mathbf{k}}^0_{\beta}\cdot\hat{\boldsymbol{\rho}}_{\alpha} = 1$ and $\epsilon_{\alpha\gamma}\hat{\mathbf{k}}^0_{\gamma}\cdot\hat{\boldsymbol{\rho}}_{\alpha} = 1$. As was shown in [24], in this whole region $\Psi^{(+)as}_{\mathbf{q}^0_{\alpha}\mathbf{k}^0_{\alpha}}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$ (i) satisfies the asymptotic Schrödinger equation (31), or equivalently the three-body Schrödinger equation (24) in Ω_{α} , up to terms of the order $O(1/\rho_{\alpha}^2)$, viz.,

$$\{E - H^{as}_{\alpha}\} \Psi^{(+)as}_{\mathbf{q}^{0}_{\alpha}\mathbf{k}^{0}_{\alpha}}(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha}) = O\left(\frac{1}{\rho^{2}_{\alpha}}\right),$$
(43)

and (ii) represents the leading term in the asymptotic expansion in Ω_{α} of the full wave function $\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$, which belongs to three asymptotically free particles in the continuum with Jacobi momenta \mathbf{k}_{α}^{0} and \mathbf{q}_{α}^{0} , viz.,

$$\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha}) = \Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha}) + O\left(\frac{1}{\rho_{\alpha}}\right).$$
(44)

The next-to-leading term in the expansion (44) satisfies (43) in the next orders. We remark that the second term in (44), which is of the order $O(1/\rho_{\alpha})$, includes rescattering of the particles β and γ from particle α [4]. Its existence can easily be deduced within the solvable model considered in [24] (which corresponds to $V_{\alpha} = 0$, $m_{\alpha} = \infty$).

2) The asymptotic Schrödinger equation (31) admits also another (exact) solution, belonging to the same energy $E = q_{\alpha}^{0^2}/2M_{\alpha} + k_{\alpha}^{0^2}/2\mu_{\alpha}$ as (37), viz.

$$\tilde{\Psi}_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha}) = \psi_{\mathbf{k}_{\alpha}^{0}}^{(+)}(\mathbf{r}_{\alpha})\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}), \qquad (45)$$

where $\psi_{\mathbf{k}_{\alpha}^{0}}^{(+)}(\mathbf{r}_{\alpha})$ is again continuum solution of the two-particle Schrödinger equation (40), but to the energy $k_{\alpha}^{0^{2}}/2\mu_{\alpha}$. However, as shown in [24] this eigenfunction of the asymptotic Hamiltonian H_{α}^{as} is not the leading term in the asymptotic expansion in Ω_{α} of the solution of the original Schrödinger equation (24), that is, it does not satisfy a relation like (44). Hence it is not to be used in the present context (as was done mistakenly in [18]).

Consequently, the asymptotic form of the spectral representation of the three-body Green function $G^Q(z)$, which is valid in $\Omega_{\alpha} \cap \Omega'_{\alpha}$ and is therefore appropriate for the investigation of the singularity structure of $\mathcal{V}^{opt\,(2)}_{\alpha m,\alpha m}$, has the form

$$G^{Q}(\boldsymbol{\rho}_{\alpha}',\mathbf{r}_{\alpha}';\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha};E+i0) \xrightarrow{\Omega_{\alpha}\cap\Omega_{\alpha}'} G^{Q\,as}(\boldsymbol{\rho}_{\alpha}',\mathbf{r}_{\alpha}';\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha};E+i0) =
 \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \left\{ \sum_{n\neq m} \frac{\psi_{\alpha n}(\mathbf{r}_{\alpha}')\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}')\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)*}(\boldsymbol{\rho}_{\alpha})\psi_{\alpha n}^{*}(\mathbf{r}_{\alpha})}{[E+i0-q_{\alpha}^{0\,2}/2M_{\alpha}-\hat{E}_{\alpha n}]} \right.
 + \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \frac{\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as}(\boldsymbol{\rho}_{\alpha}',\mathbf{r}_{\alpha}')\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as*}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})}{[E+i0-q_{\alpha}^{0\,2}/2M_{\alpha}-k_{\alpha}^{0\,2}/2\mu_{\alpha}]} \right\}.$$
(46)

One last point concerns the fact that in the second term on the r.h.s. of (46) the integrations over \mathbf{q}^0_{α} and \mathbf{k}^0_{α} extend also over the singular directions, i.e., directions such that $\epsilon_{\alpha\beta}\hat{\mathbf{k}}^0_{\beta}\cdot\hat{\boldsymbol{\rho}}_{\alpha} = 1$ and $\epsilon_{\alpha\gamma}\hat{\mathbf{k}}^0_{\gamma}\cdot\hat{\boldsymbol{\rho}}_{\alpha} = 1$ holds. But there, as mentioned above, the asymptotic expansion (44) is not valid. Thus, in principle in the vicinity of these directions the exact expression of the three-body wave function $\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$ must be used, which is however unknown. Since the latter is normalized to $\delta(\mathbf{q}^0_{\alpha} - \mathbf{q}^{0'}_{\alpha})\delta(\mathbf{k}^0_{\alpha} - \mathbf{k}^{0'}_{\alpha})$, it has to be integrable everywhere, including the singular directions. The consequence is that the contribution from the infinitely small regions containing the singular directions is infinitely small [28]. Thus, when looking for the asymptotic behavior of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\mathbf{q}'_{\alpha},\mathbf{q}_{\alpha};E)$ for $\Delta_{\alpha} \to 0$, in the main order we can approximate the exact wave function $\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$ by $\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$ in the whole integration region, including the singular directions. Of course, some care must be taken before using expression (37) in the singular directions since, as follows from its definition (42), $\mathbf{a}_{\alpha}(\hat{\boldsymbol{\rho}}_{\alpha})$ diverges there. One possible remedy has been proposed in the Appendix of ref. [24]. It consists in writing $\mathbf{a}_{\alpha}(\hat{\boldsymbol{\rho}}_{\alpha})/\rho_{\alpha} \approx$ $i \sum_{\nu=\beta,\gamma} \epsilon_{\alpha\nu} \lambda_{\nu} \nabla \boldsymbol{\rho}_{\alpha} \ln F(-i\eta_{\nu}, 1; i(k_{\nu}\rho_{\alpha} - \epsilon_{\alpha\nu}\mathbf{k}_{\nu} \cdot \boldsymbol{\rho}_{\alpha})).$ The right-hand side has the virtue of remaining regular when the singular directions are approached, while away from them it coincides for $\rho_{\alpha} \to \infty$ in leading order with the right-hand side of (42).

Summarizing, higher order terms in the expansion (44) will not contribute to the leading term of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\mathbf{q}'_{\alpha},\mathbf{q}_{\alpha};E)$ in the limit $\Delta_{\alpha} \to 0$, because its behavior is defined by the divergence of the integrals over $\boldsymbol{\rho}'_{\alpha}$ and $\boldsymbol{\rho}_{\alpha}$ in (23) for $\boldsymbol{\rho}'_{\alpha}, \boldsymbol{\rho}_{\alpha} \to \infty$. And the contribution from the infinitely small neighbourhoods of the singular directions is infinitely small. Thus we can use the representation (46) everywhere.

As discussed above, in Ω_{α} the potentials V_{β} and V_{γ} occurring in (23) can in the main order in $1/\rho_{\alpha}$ be approximated by their Coulombic parts V_{β}^{C} and V_{γ}^{C} . The same holds true in Ω'_{α} . Thus, in the limit $\Delta_{\alpha} \to 0$ one gets for the leading, Δ_{α} -dependent part $\mathcal{V}^{opt}_{\alpha m,\alpha m}$ of the optical potential term $\mathcal{V}^{opt}_{\alpha m,\alpha m}^{(2)}$:

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to0}{\approx} \mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \\ = \sum_{\mu,\nu} \bar{\delta}_{\nu\alpha} \bar{\delta}_{\mu\alpha} \int_{\rho_{\alpha}'\geq A} d\boldsymbol{\rho}_{\alpha}' \, d\mathbf{r}_{\alpha}' \, \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} \, d\mathbf{r}_{\alpha}$$

$$\times \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} e^{-i\mathbf{q}_{\alpha}'\cdot\boldsymbol{\rho}_{\alpha}'} \psi_{\alpha m}^{*}(\mathbf{r}_{\alpha}') V_{\mu}^{C}(\epsilon_{\alpha\mu}\boldsymbol{\rho}_{\alpha}'-\lambda_{\mu}\mathbf{r}_{\alpha}')$$

$$\times \left\{ \sum_{n\neq m} \frac{\psi_{\alpha n}(\mathbf{r}_{\alpha}')\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}')\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)*}(\boldsymbol{\rho}_{\alpha})\psi_{\alpha n}^{*}(\mathbf{r}_{\alpha})}{[E+i0-q_{\alpha}^{0\,2}/2M_{\alpha}-\hat{E}_{\alpha n}]} + \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \frac{\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as}(\boldsymbol{\rho}_{\alpha}',\mathbf{r}_{\alpha}')\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as*}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})}{[E+i0-q_{\alpha}^{0\,2}/2M_{\alpha}-k_{\alpha}^{0\,2}/2\mu_{\alpha}]} \right\}$$

$$\times V_{\nu}^{C}(\epsilon_{\alpha\nu}\boldsymbol{\rho}_{\alpha}-\lambda_{\nu}\mathbf{r}_{\alpha})\psi_{\alpha m}(\mathbf{r}_{\alpha})e^{i\mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}}. \tag{47}$$

The radius A, which defines the lower limits in the integrals over the magnitudes of ρ'_{α} and ρ_{α} , has to be chosen so large that $A \gg 1/\kappa_{\alpha m}$, with $\kappa_{\alpha m}$ defined previously. This condition ensures that we are allowed to use the asymptotic expansion (44) and to replace the full two-body potentials by their Coulombic parts. These approximations have already been introduced in (47).

III. BEHAVIOR OF THE OPTICAL POTENTIAL IN THE LIMIT OF VANISHING MOMENTUM TRANSFER

In this section we will make use of techniques and results developed for an analogous problem in two-particle scattering in [28]. In Ω_{α} we can use the asymptotic expansion

$$V_{\nu}^{C}(\epsilon_{\alpha\nu}\boldsymbol{\rho}_{\alpha}-\lambda_{\nu}\mathbf{r}_{\alpha})=\frac{e_{\tilde{\nu}}e_{\alpha}}{\rho_{\alpha}}+\epsilon_{\alpha\nu}\lambda_{\nu}\frac{e_{\tilde{\nu}}e_{\alpha}}{\rho_{\alpha}^{2}}(\hat{\boldsymbol{\rho}}_{\alpha}\cdot\mathbf{r}_{\alpha})+O\left(\frac{r_{\alpha}^{2}}{\rho_{\alpha}^{3}}\right),\quad\text{with}\quad\nu\neq\tilde{\nu}=\beta,\gamma.$$
 (48)

For the following it proves useful to apply the familiar screening to the Coulomb potentials which we choose to be of exponential type in coordinate space, i.e., $V_{\alpha}^{C}(\mathbf{r}_{\alpha}) \rightarrow V_{\alpha}^{C}(\mathbf{r}_{\alpha})e^{-\delta r_{\alpha}}$, $\delta > 0$. The zero-screening limit $\delta \rightarrow +0$ will then be taken at the end. Substitute (37) and (48) into (47). The orthogonality of the bound state wave function $\psi_{\alpha m}(\mathbf{r}_{\alpha})$ to all the other bound state wave functions $\psi_{\alpha n}(\mathbf{r}_{\alpha})$ for $n \neq m$ and to the scattering wave functions $\psi_{\mathbf{k}_{\alpha}^{(1)}(\boldsymbol{\rho}_{\alpha})}^{(1)}(\mathbf{r}_{\alpha})$ causes the vanishing of the contribution of the first term of the expansion (48). Thus one obtains in leading order for $\Delta_{\alpha} \rightarrow 0$:

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to0}{\approx} \lim_{\delta\to+0} \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \int_{\rho_{\alpha}'\geq A} d\boldsymbol{\rho}_{\alpha}' \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} \frac{e^{-i(\mathbf{q}_{\alpha}'-\mathbf{q}_{\alpha}^{0})\cdot\boldsymbol{\rho}_{\alpha}'}}{\rho_{\alpha}'^{2}} e^{-\delta\rho_{\alpha}'} \\
\times \left\{ \tilde{\psi}_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}') \sum_{n\neq m} \frac{D_{mn}(\hat{\boldsymbol{\rho}}_{\alpha})D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha})}{[E+i0-q_{\alpha}^{0\,2}/2M_{\alpha}-\hat{E}_{\alpha n}]} \tilde{\psi}_{\mathbf{q}_{\alpha}^{0}}^{(+)*}(\boldsymbol{\rho}_{\alpha}) \\
+ \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \prod_{\nu=\beta,\gamma} e^{i\eta_{\nu}^{0}\ln(k_{\nu}^{0}\rho_{\alpha}'-\mathbf{k}_{\nu}^{0}\cdot\boldsymbol{\rho}_{\alpha}')} \prod_{\sigma=\beta,\gamma} e^{-i\eta_{\sigma}^{0}\ln(k_{\sigma}^{0}\rho_{\alpha}-\mathbf{k}_{\sigma}^{0}\cdot\boldsymbol{\rho}_{\alpha})} \\
\times \frac{D_{m\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha}')(\hat{\boldsymbol{\rho}}_{\alpha}')D_{\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})m(\hat{\boldsymbol{\rho}}_{\alpha})}{[E+i0-q_{\alpha}^{0\,2}/2M_{\alpha}-k_{\alpha}^{0\,2}/2\mu_{\alpha}]} \right\} e^{-\delta\rho_{\alpha}} \frac{e^{i(\mathbf{q}_{\alpha}-\mathbf{q}_{\alpha}^{0})\cdot\boldsymbol{\rho}_{\alpha}}}{\rho_{\alpha}^{2}}, \quad (49)$$

where we have introduced

$$D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha}) = \epsilon_{\alpha\beta} e_{\alpha} (\lambda_{\beta} e_{\gamma} - \lambda_{\gamma} e_{\beta}) \int d\mathbf{r}_{\alpha} \psi_{\alpha n}^{*}(\mathbf{r}_{\alpha}) (\hat{\boldsymbol{\rho}}_{\alpha} \cdot \mathbf{r}_{\alpha}) \psi_{\alpha m}(\mathbf{r}_{\alpha}), \tag{50}$$

$$D_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})m}(\hat{\boldsymbol{\rho}}_{\alpha}) = \epsilon_{\alpha\beta}e_{\alpha}(\lambda_{\beta}e_{\gamma} - \lambda_{\gamma}e_{\beta}) \int d\mathbf{r}_{\alpha}\psi_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})}^{(+)*}(\mathbf{r}_{\alpha})(\hat{\boldsymbol{\rho}}_{\alpha}\cdot\mathbf{r}_{\alpha})\psi_{\alpha m}(\mathbf{r}_{\alpha}), \tag{51}$$

$$D_{mn}(\hat{\boldsymbol{\rho}}_{\alpha}) = D_{nm}^{*}(\hat{\boldsymbol{\rho}}_{\alpha}), \quad D_{m\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})}(\hat{\boldsymbol{\rho}}_{\alpha}) = D_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})m}^{*}(\hat{\boldsymbol{\rho}}_{\alpha}).$$
(52)

For convenience, the plane wave has been extracted in (49) from the center-of-mass Coulomb wave function (35), by writing $\psi_{\mathbf{q}_{\alpha}^{(+)}}^{(+)}(\boldsymbol{\rho}_{\alpha}) = e^{i\mathbf{q}_{\alpha}^{0}\cdot\boldsymbol{\rho}_{\alpha}}\tilde{\psi}_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}).$

Inspection of (49) reveals that the integrals over ρ'_{α} and ρ_{α} will diverge for $\rho'_{\alpha}, \rho_{\alpha} \to \infty$ if and only if $(\mathbf{q}'_{\alpha} - \mathbf{q}^0_{\alpha})^2 \to -\delta^2$ and $(\mathbf{q}_{\alpha} - \mathbf{q}^0_{\alpha})^2 \to -\delta^2$, respectively. These divergences will give rise to singularities in the integrand of the final \mathbf{q}^0_{α} -integration at the positions

$$(\mathbf{q}'_{\alpha} - \mathbf{q}^{0}_{\alpha})^{2} + \delta^{2} = 0 \quad \text{and} \quad (\mathbf{q}_{\alpha} - \mathbf{q}^{0}_{\alpha})^{2} + \delta^{2} = 0.$$
(53)

For $\delta \to +0$ we get from (53) for the positions of the singularities

$$\mathbf{q}^0_\alpha = \mathbf{q}'_\alpha, \quad \mathbf{q}^0_\alpha = \mathbf{q}_\alpha. \tag{54}$$

Proceeding then in close analogy to [28], it will be shown below that the coincidence of these singularities when integrating over \mathbf{q}^0_{α} gives rise to a singularity of $\mathcal{V}^{opt\,(as)}_{\alpha m,\alpha m}$ in the limit $\Delta_{\alpha} \to 0$ of the form

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{\sim} \Delta_{\alpha} = \sqrt{q_{\alpha}'^{2} + q_{\alpha}^{2} - 2q_{\alpha}'q_{\alpha}z}$$

$$\stackrel{q_{\alpha}'\to q_{\alpha}}{\sim} \sqrt{1-z}, \quad z = \hat{\mathbf{q}}_{\alpha}' \cdot \hat{\mathbf{q}}_{\alpha}. \tag{55}$$

That is, $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}$ has a singularity in the forward direction at z = 1 in the z-plane which defines the behavior of the leading term in the limit $z \to 1$, or equivalently $\Delta_{\alpha} \to 0$.

From (54) we can conclude that in the limit $\Delta_{\alpha} \to 0$ the main contribution to the integral over \mathbf{q}^{0}_{α} comes from the neighbourhood

$$\mathbf{q}^0_\alpha \approx \mathbf{q}_\alpha \approx \mathbf{q}'_\alpha. \tag{56}$$

In [28] this has been proved in the case of two-body scattering, but it holds also for the three-body case considered here. For, the additional integration over \mathbf{k}^{0}_{α} appearing in the intermediate three-body continuum state contribution in (49) does not influence this conclusion. Thus the leading singular behavior of $\mathcal{V}^{opt\,(as)}_{\alpha m,\alpha m}$ is defined by the divergence of the integrals over $\boldsymbol{\rho}_{\alpha}$, over $\boldsymbol{\rho}'_{\alpha}$, and over \mathbf{q}^{0}_{α} .

A. Contribution from two-fragment intermediate states

Let us first consider that part of (49) which is due to the contribution from all subsystem bound states $n \neq m$ in the intermediate state,

$$\mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to0}{\approx} \lim_{\delta\to+0} \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \int_{\rho_{\alpha}'\geq A} d\boldsymbol{\rho}_{\alpha} \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} \frac{e^{-i\mathbf{q}_{\alpha}'\cdot\boldsymbol{\rho}_{\alpha}'}}{\rho_{\alpha}'^{2}} e^{-\delta\rho_{\alpha}'} \psi_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}') \\ \times \sum_{n\neq m} \frac{D_{mn}(\hat{\boldsymbol{\rho}}_{\alpha}')D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha})}{[q_{\alpha n}^{2}/2M_{\alpha}+i0-q_{\alpha}^{0}^{2}/2M_{\alpha}]} \psi_{\mathbf{q}_{\alpha}^{0}}^{(+)*}(\boldsymbol{\rho}_{\alpha}) e^{-\delta\rho_{\alpha}} \frac{e^{i\mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}}}{\rho_{\alpha}^{2}}.$$
 (57)

Since the behavior of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}$ for $\Delta_{\alpha} \to 0$ is determined by momenta characterized by (56), the propagator

$$d_n(q_{\alpha}^0) = \left[E + i0 - q_{\alpha}^{0^2}/2M_{\alpha} - \hat{E}_{\alpha n}\right]^{-1}$$
(58)

can be taken out from under the integral over \mathbf{q}^0_{α} at the point $q^0_{\alpha} = q_{\alpha}$, provided it is not singular there. Let us write (58) as

$$d_n(q^0_{\alpha}) = 2M_{\alpha} / \left[q^2_{\alpha n} - q^{0^2}_{\alpha} + i0 \right],$$
(59)

with (recall (9))

$$q_{\alpha n}^{2} = 2M_{\alpha}(E - \hat{E}_{\alpha n}) = \bar{q}_{\alpha}^{2} + 2M_{\alpha}(\hat{E}_{\alpha m} - \hat{E}_{\alpha n}), \quad n \neq m.$$
(60)

If $\mathbf{q}_{\alpha}^{0} = \mathbf{q}_{\alpha}$, then for on-shell scattering, i.e. for $q_{\alpha} = \bar{q}_{\alpha}$, $d_{n}(q_{\alpha})$ is always finite. However, for off-shell scattering $(q_{\alpha} \neq \bar{q}_{\alpha})$, $d_{n}(q_{\alpha})$ has for $E - \hat{E}_{\alpha n} > 0$ a pole at $q_{\alpha} = q_{\alpha n}$. This pole occurs both for E > 0 and for E < 0, i.e. for energies above and below the dissociation threshold.

Summarizing, for $q_{\alpha}^{0} = q_{\alpha} \neq q_{\alpha n}$, $d_{n}(q_{\alpha}^{0})$ is not singular and can therefore be taken out from under the integral over \mathbf{q}_{α}^{0} at the momentum $q_{\alpha}^{0} = q_{\alpha}$ when trying to extract the behavior of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}$ in the limit $\Delta_{\alpha} \to 0$ in leading order [28]. Clearly this is no longer allowed at the point $q_{\alpha} = q_{\alpha n}$ where the propagator $d_{n}(q_{\alpha})$ has a pole.

Thus, if $q_{\alpha} \neq q_{\alpha n}$, we have in leading order

$$\mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to0}{\approx} \sum_{n\neq m} \frac{2M_{\alpha}}{q_{\alpha n}^{2}-q_{\alpha}^{2}} \lim_{\delta\to+0} \int_{\rho_{\alpha}'\geq A} d\boldsymbol{\rho}_{\alpha}' \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha}' \frac{e^{-i\mathbf{q}_{\alpha}'\cdot\boldsymbol{\rho}_{\alpha}'}}{\rho_{\alpha}'^{2}} e^{-\delta\rho_{\alpha}'} D_{mn}(\hat{\boldsymbol{\rho}}_{\alpha}') \\ \times D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha}) e^{-\delta\rho_{\alpha}} \frac{e^{i\mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}}}{\rho_{\alpha}^{2}} \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \left\{ \psi_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}')\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)*}(\boldsymbol{\rho}_{\alpha}) \right\}.$$
(61)

We can use the completeness relation

$$\int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \left\{ \psi_{\mathbf{q}_{\alpha}^{0}}^{(+)}(\boldsymbol{\rho}_{\alpha}')\psi_{\mathbf{q}_{\alpha}^{0}}^{(+)*}(\boldsymbol{\rho}_{\alpha}) \right\} = \delta(\boldsymbol{\rho}_{\alpha}'-\boldsymbol{\rho}_{\alpha}) - \sum_{\kappa}\psi_{\kappa}(\boldsymbol{\rho}_{\alpha}')\psi_{\kappa}^{*}(\boldsymbol{\rho}_{\alpha}), \tag{62}$$

for the solutions of (34). Of course, if the center-of-mass Coulomb potential $v_{\alpha}^{C}(\boldsymbol{\rho}_{\alpha})$ is repulsive, the sum over all bound states κ with wave functions $\psi_{\kappa}(\boldsymbol{\rho}_{\alpha})$ is missing. Introducing (62) into (61) we obtain

$$\mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{\approx} \sum_{n\neq m} \frac{2M_{\alpha}}{q_{\alpha n}^2 - q_{\alpha}^2} \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} \frac{e^{-i\boldsymbol{\Delta}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}}}{\rho_{\alpha}^4} |D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha})|^2.$$
(63)

To arrive at this expression we have already taken into account that, owing to the presence of the factor ρ_{α}^{-4} in the integrand, the integral in (63) converges, so that the limit $\delta \to +0$ and the integration over ρ_{α} could be interchanged.

In fact, the result (63) is valid both for repulsive and attractive center-of-mass Coulomb potentials. For, when deriving it for the latter case, one only has to bear in mind that the bound state part in (62), when inserted in (61), gives rise to terms in which the integrals over ρ_{α} and ρ'_{α} do not diverge for $\rho_{\alpha}, \rho'_{\alpha} \to \infty$, due to the exponential decay of the bound state wave functions, and thus lead to nonsingular expressions. Furthermore, each of these terms is separable with respect to \mathbf{q}_{α} and \mathbf{q}'_{α} ; thus they can not contribute at all to the momentum-transfer dependence of $\mathcal{V}^{opt\,(as)}_{\alpha m,\alpha m\,(b)}$ in the limit $\Delta_{\alpha} \to 0$.

In the case $q_{\alpha} = q_{\alpha n}$, the propagator $d_n(q_{\alpha}^0)$ can not be taken out from under the integral over \mathbf{q}_{α}^0 at the point $q_{\alpha}^0 = q_{\alpha}$. This implies that at the discrete points $q_{\alpha} = q_{\alpha n}$, $n \neq m$, which are accessible in off-shell scattering only, the limit $\Delta_{\alpha} \to 0$ in $\mathcal{V}_{\alpha m,\alpha m(b)}^{opt (as)}$ requires special considerations. This investigation is deferred to Appendix A where it is shown that at these discrete momenta $\mathcal{V}_{\alpha m,\alpha m(b)}^{opt (as)}$ remains regular in the limit $\Delta_{\alpha} \to 0$.

It is now an easy task to extract the behavior of (63) for $\Delta_{\alpha} \to 0$. To this end we write (50) in the form

$$D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha}) = \hat{\boldsymbol{\rho}}_{\alpha} \cdot \mathbf{D}_{nm} = \frac{i}{\rho_{\alpha}} \lim_{\mathbf{p} \to 0} (\mathbf{D}_{nm} \cdot \boldsymbol{\nabla}_{\mathbf{p}}) e^{-i\mathbf{p} \cdot \boldsymbol{\rho}_{\alpha}}, \tag{64}$$

with

$$\mathbf{D}_{nm} = \epsilon_{\alpha\beta} e_{\alpha} (\lambda_{\beta} e_{\gamma} - \lambda_{\gamma} e_{\beta}) \int d\mathbf{r}_{\alpha} \psi_{\alpha n}^{*}(\mathbf{r}_{\alpha}) \mathbf{r}_{\alpha} \psi_{\alpha m}(\mathbf{r}_{\alpha}), \qquad (65)$$

and use the symmetry property (52). Then

$$\mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{\approx} \sum_{n\neq m} \frac{2M_{\alpha}}{q_{\alpha n}^2 - q_{\alpha}^2} \lim_{\mathbf{p},\mathbf{p}'\to 0} (\mathbf{D}_{mn}\cdot\boldsymbol{\nabla}_{\mathbf{p}'})(\mathbf{D}_{nm}\cdot\boldsymbol{\nabla}_{\mathbf{p}})J(\mathbf{u}), \tag{66}$$

the integral $J(\mathbf{u})$ being defined as

$$J(\mathbf{u}) = \int_{\rho_{\alpha} \ge \mathbf{A}} \mathrm{d}\boldsymbol{\rho}_{\alpha} \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{\rho}_{\alpha} \cdot \mathbf{u}}}{\rho_{\alpha}^{6}} = \frac{4\pi}{\mathrm{u}} \int_{\mathbf{A}}^{\infty} \mathrm{d}\rho_{\alpha} \frac{\sin \mathrm{u}\rho_{\alpha}}{\rho_{\alpha}^{5}},\tag{67}$$

with $\mathbf{u} = \mathbf{p}' - \mathbf{\Delta}_{\alpha} - \mathbf{p}$. This integral is evaluated in Appendix B. Substituting its asymptotic form (B.3) for $u \to 0$ (i.e. \mathbf{p}', \mathbf{p} , and Δ_{α} going to zero) into (66) leads to

$$\mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{=} C_{m}^{(b)}\Delta_{\alpha} + o\,(\Delta_{\alpha}),\tag{68}$$

with

$$C_m^{(b)} = -\frac{\pi^2}{2} \sum_{n \neq m} \frac{M_\alpha}{q_{\alpha n}^2 - q_\alpha^2} \left[|\mathbf{D}_{nm}|^2 + |\hat{\mathbf{\Delta}}_\alpha \cdot \mathbf{D}_{nm}|^2 \right].$$
(69)

We mention that the action of $\nabla_{\mathbf{p}'}$ and $\nabla_{\mathbf{p}}$ onto the term $\sim u^2$ in the asymptotic form (B.3) for $J(\mathbf{u})$ yields in the limit $\mathbf{p}, \mathbf{p}' \to 0$ also a Δ_{α} -independent term. The latter was, however, omitted in (68) since $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}$ was defined as the leading, Δ_{α} -dependent contribution from the intermediate two-fragment states to the nontrivial part $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(2)}$ of the optical potential in the limit $\Delta_{\alpha} \to 0$.

For on-shell scattering $(q'_{\alpha} = q_{\alpha} = \bar{q}_{\alpha})$ we have

$$(q_{\alpha n}^2 - q_{\alpha}^2)/2M_{\alpha} = \hat{E}_{\alpha m} - \hat{E}_{\alpha n}, \quad n \neq m,$$
(70)

and hence (69) becomes

$$C_m^{(b)} = -\frac{\pi^2}{4} \sum_{n \neq m} \frac{1}{\hat{E}_{\alpha m} - \hat{E}_{\alpha n}} \left[|\mathbf{D}_{nm}|^2 + |\hat{\mathbf{\Delta}}_{\alpha} \cdot \mathbf{D}_{nm}|^2 \right].$$
(71)

Thus, $\mathcal{V}_{\alpha m,\alpha m(b)}^{opt\,(as)}$ as given by (68) and (71), depends only on the momentum transfer Δ_{α} , and not on the incoming or outgoing momentum \mathbf{q}_{α} and \mathbf{q}'_{α} separately, or on the energy. Consequently, on the energy shell we can write (63) as

$$\mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E_{\alpha m}+i0) \equiv \mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\boldsymbol{\Delta}_{\alpha})$$

$$\stackrel{\Delta_{\alpha}\to 0}{\approx} \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} e^{-i\boldsymbol{\Delta}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} \mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\boldsymbol{\rho}_{\alpha}), \qquad (72)$$

where

$$\mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}(\boldsymbol{\rho}_{\alpha}) = \left(\sum_{n \neq m} \frac{|D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha})|^2}{\hat{E}_{\alpha m} - \hat{E}_{\alpha n}}\right) \frac{1}{\rho_{\alpha}^4} \tag{73}$$

describes the asymptotics of $\mathcal{V}_{\alpha m,\alpha m\,(b)}^{opt\,(as)}$ in the coordinate space. It is a local potential, representing the contribution to the polarisation potential from all the intermediate two-fragment states.

B. Contribution from intermediate three-particle continuum states

We now proceed to investigate the contribution $\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}$ of the intermediate threeparticle continuum states to the optical potential, which is given by the integral part in the wavy brackets of (49), in the limit $\Delta_{\alpha} \to 0$:

$$\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to0}{\approx} \lim_{\delta\to+0} \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha}' \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} \frac{e^{-i(\mathbf{q}_{\alpha}'-\mathbf{q}_{\alpha}^{0})\cdot\boldsymbol{\rho}_{\alpha}'}}{\rho_{\alpha}'^{2}} e^{-\delta\rho_{\alpha}'} \times e^{-\delta\rho_{\alpha}} \frac{e^{i(\mathbf{q}_{\alpha}-\mathbf{q}_{\alpha}^{0})\cdot\boldsymbol{\rho}_{\alpha}}}{\rho_{\alpha}^{2}} L(\mathbf{q}_{\alpha}^{0};\boldsymbol{\rho}_{\alpha},\boldsymbol{\rho}_{\alpha}'),$$
(74)

with

$$L(\mathbf{q}_{\alpha}^{0};\boldsymbol{\rho}_{\alpha},\boldsymbol{\rho}_{\alpha}') = \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \prod_{\nu=\beta,\gamma} e^{i\eta_{\nu}^{0}\ln(k_{\nu}^{0}\rho_{\alpha}'-\mathbf{k}_{\nu}^{0}\cdot\boldsymbol{\rho}_{\alpha}')} \prod_{\sigma=\beta,\gamma} e^{-i\eta_{\sigma}^{0}\ln(k_{\sigma}^{0}\rho_{\alpha}-\mathbf{k}_{\sigma}^{0}\cdot\boldsymbol{\rho}_{\alpha})} \times \frac{D_{m\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha}')D_{\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})m(\hat{\boldsymbol{\rho}}_{\alpha})}{[E+i0-q_{\alpha}^{0^{2}}/2M_{\alpha}-k_{\alpha}^{0^{2}}/2\mu_{\alpha}]}.$$
(75)

Consider the integration over \mathbf{q}_{α}^{0} in (74). Since, as discussed above, the behavior of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}$ for $\Delta_{\alpha} \to 0$ is defined by momenta characterized by the restriction (56), the function $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ can be taken out from under the integral over \mathbf{q}_{α}^{0} at the momentum $\mathbf{q}_{\alpha}^{0} = \mathbf{q}_{\alpha}$ provided it is nonsingular there. A singularity of L in the \mathbf{q}_{α}^{0} -plane, which may be of concern to us in the present context, can be generated in (75) only by the pole of the propagator

$$d_{k_{\alpha}^{0}}(q_{\alpha}^{0}) = \left[E + i0 - q_{\alpha}^{0^{2}}/2M_{\alpha} - k_{\alpha}^{0^{2}}/2\mu_{\alpha}\right]^{-1}$$
(76)

 k_{α}^{0} -plane. In fact, this pole induces in the function $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ a singularity in the q_{α}^{0} -plane at $q_{\alpha}^{0} = \sqrt{2M_{\alpha}E}$ (the positive square root is singled out by the infinitely small imaginary part +i0 in the propagator). It is an end point singularity which results from the coincidence of the propagator pole with the lower limit zero of the integration over k_{α}^{0} .

Hence one has to distinguish two cases.

(i) $q_{\alpha} \neq \sqrt{2M_{\alpha}E}$, i.e., the function $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ is regular at the momentum $\mathbf{q}_{\alpha}^{0} = \mathbf{q}_{\alpha}$ (this is obvious since the propagator pole at $k_{\alpha}^{0} = \sqrt{2\mu_{\alpha}(E - q_{\alpha}^{2}/2M_{\alpha})} \neq 0$ does not coincide with the lower limit $k_{\alpha}^{0} = 0$ of the integration in (75)). As a consequence, $L(\mathbf{q}^0_{\alpha}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}'_{\alpha})$ can be taken out from under the integral over \mathbf{q}^0_{α} at $\mathbf{q}^0_{\alpha} = \mathbf{q}_{\alpha}$ when looking for the behavior of $\mathcal{V}^{opt\,(as)}_{\alpha m,\alpha m\,(c)}$ in the limit $\Delta_{\alpha} \to 0$. This holds true *a fortiori* for the propagator $d_{k^0_{\alpha}}(q^0_{\alpha})$ in (75). For $q^0_{\alpha} = q_{\alpha}$, the latter can be written as (recall (9))

$$d_{k_{\alpha}^{0}}(q_{\alpha}) = \left[\bar{q}_{\alpha}^{2}/2M_{\alpha} - q_{\alpha}^{2}/2M_{\alpha} - k_{\alpha}^{0^{2}}/2\mu_{\alpha} + \hat{E}_{\alpha m} + i0\right]^{-1}.$$
(77)

Note that on the energy shell, i.e., for $q_{\alpha} = \bar{q}_{\alpha}$, expression (77) simplifies to

$$d_{k_{\alpha}^{0}}(q_{\alpha}) = -\left[|\hat{E}_{\alpha m}| + k_{\alpha}^{0^{2}}/2\mu_{\alpha}\right]^{-1} < 0,$$
(78)

that is, the propagator $d_{k^0_\alpha}(q^0_\alpha)$ is nonsingular at $q^0_\alpha = q_\alpha = \bar{q}_\alpha$ for all k^0_α .

(ii) $q_{\alpha} = \sqrt{2M_{\alpha}E}$, which can happen only off the energy shell for E > 0. In this case $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ cannot be taken out from under the integral over \mathbf{q}_{α}^{0} in (74) at the point $\mathbf{q}_{\alpha}^{0} = \mathbf{q}_{\alpha}$ because it is singular there. A closer examination, which is deferred to Appendix A, reveals that in the limit $\Delta_{\alpha} \to 0$, $\mathcal{V}_{\alpha m,\alpha m(c)}^{opt\,(as)}$ is $O(\Delta_{\alpha})$ if the Coulomb potential V_{α}^{C} is repulsive, and that it remains regular for an attractive Coulomb potential V_{α}^{C} . In other words, the leading singular behavior is unaltered as compared to case (i).

Summarizing, in order to isolate the leading singular part of $\mathcal{V}_{\alpha m,\alpha m(c)}^{opt\,(as)}$ for $q_{\alpha} \neq \sqrt{2M_{\alpha}E}$, we can take in (74) the propagator $d_{k_{\alpha}^{0}}(q_{\alpha}^{0})$, as well as all other q_{α}^{0} -depending factors none of which becomes singular there, out from under the integral over \mathbf{q}_{α}^{0} at the point $q_{\alpha}^{0} = q_{\alpha}$. This gives

$$\mathcal{V}_{\alpha m,\alpha m(c)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to0}{\approx} \lim_{\delta\to+0} \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \int_{\rho_{\alpha}\geq A} d\rho_{\alpha} \frac{e^{-i\mathbf{q}_{\alpha}'\cdot\boldsymbol{\rho}_{\alpha}'}}{\rho_{\alpha}'^{2}} e^{-\delta\rho_{\alpha}'} \\
\times \prod_{\nu=\beta,\gamma} \left(\frac{\bar{k}_{\nu}^{0}\rho_{\alpha}' - \bar{\mathbf{k}}_{\nu}^{0}\cdot\boldsymbol{\rho}_{\alpha}'}{\bar{k}_{\nu}^{0}\rho_{\alpha} - \bar{\mathbf{k}}_{\nu}^{0}\cdot\boldsymbol{\rho}_{\alpha}} \right)^{i\bar{\eta}_{\nu}^{0}} e^{-\delta\rho_{\alpha}} \frac{e^{i\mathbf{q}_{\alpha}}\cdot\boldsymbol{\rho}_{\alpha}}{\rho_{\alpha}^{2}} \\
\times \frac{D_{m\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha}')(\hat{\boldsymbol{\rho}}_{\alpha}')D_{\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})m(\hat{\boldsymbol{\rho}}_{\alpha})}{[E+i0-q_{\alpha}^{2}/2M_{\alpha}-k_{\alpha}^{0^{2}}/2\mu_{\alpha}]} \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} e^{i\mathbf{q}_{\alpha}^{0}\cdot(\boldsymbol{\rho}_{\alpha}'-\boldsymbol{\rho}_{\alpha})} \\
= \lim_{\delta\to+0} \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} \frac{e^{-i\Delta_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}}}{\rho_{\alpha}^{4}} e^{-2\delta\rho_{\alpha}} \\
\times \frac{D_{m\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})(\hat{\boldsymbol{\rho}}_{\alpha})D_{\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})m(\hat{\boldsymbol{\rho}}_{\alpha})}{[E+i0-q_{\alpha}^{2}/2M_{\alpha}-k_{\alpha}^{0^{2}}/2\mu_{\alpha}]},$$
(79)

where $\bar{\mathbf{k}}_{\nu}^{0}$ is given by the relation (39), but with \mathbf{q}_{α} instead of \mathbf{q}_{α}^{0} . Similarly, $\bar{\eta}_{\nu}^{0}$ is defined as in (38), but with $\bar{\mathbf{k}}_{\nu}^{0}$ instead of \mathbf{k}_{ν}^{0} .

We remark that the fact that the leading term of (74) for $\Delta_{\alpha} \to 0$ is defined by that part of the integration region where $\rho'_{\alpha} = \rho_{\alpha}$, was derived for an analogous two-body problem in [28]. As is apparent, the additional integration over \mathbf{k}^{0}_{α} , which is present in the three-body case under consideration, does not invalidate that result.

Next we observe that, since the behavior of $\mathcal{V}_{\alpha m,\alpha m(c)}^{opt(as)}$ for $\Delta_{\alpha} \to 0$ is defined by the behavior of the integrand in (79) for $\rho_{\alpha} \to \infty$, we can approximate $D_{\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})_{m}(\hat{\boldsymbol{\rho}}_{\alpha})$ by $D_{\mathbf{k}_{\alpha}^{0}m}(\hat{\boldsymbol{\rho}}_{\alpha})$, i.e. by the same expression (51) but with the local momentum $\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})$ replaced by its asymptotic value \mathbf{k}_{α}^{0} which is attained in this limit. In fact, taking into account (51), (40) and (41) one sees that

$$D_{\mathbf{k}^{0}_{\alpha}(\boldsymbol{\rho}_{\alpha})m}(\hat{\boldsymbol{\rho}}_{\alpha}) = D_{\mathbf{k}^{0}_{\alpha}m}(\hat{\boldsymbol{\rho}}_{\alpha}) + O\left(\frac{1}{\rho_{\alpha}}\right).$$
(80)

An analogous expansion applies to $D_{m\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})(\hat{\boldsymbol{\rho}}_{\alpha})$. It is important to realize that (80) is valid for any $k_{\alpha}^{0} > 0$: for arbitrary positive-definite k_{α}^{0} always such a large A can be found that for all $\rho_{\alpha} \geq A$ the second term in (80) is infinitely small compared to the first one. This obviously does no longer hold true for $k_{\alpha}^{0} = 0$, as follows from the definition (41) of the local momentum. But the whole integral is not influenced by the behavior of the integrand in an infinitesimal vicinity of $k_{\alpha}^{0} = 0$ if the latter does not possess a nonintegrable singularity there. This is verified in Appendix A for $q_{\alpha} \neq \sqrt{2M_{\alpha}E}$. Thus we are justified in using the approximation (80) in the whole region of integration over \mathbf{k}_{α}^{0} including the origin, thereby neglecting the terms of the order $O(1/\rho_{\alpha})$.

Introducing (80) in (79) yields in the leading order

$$\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{\approx} \int_{\rho_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} \frac{e^{-i\boldsymbol{\Delta}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}}}{\rho_{\alpha}^{4}} \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \frac{|D_{\mathbf{k}_{\alpha}^{0}m}(\hat{\boldsymbol{\rho}}_{\alpha})|^{2}}{[E+i0-q_{\alpha}^{2}/2M_{\alpha}-k_{\alpha}^{0}/2\mu_{\alpha}]}$$
(81)

(again, because of the convergence factor ρ_{α}^{-4} the limit $\delta \to +0$ could be performed before integrating over ρ_{α}).

Let us write, in analogy to (64),

$$D_{\mathbf{k}_{\alpha}^{0}m}(\hat{\boldsymbol{\rho}}_{\alpha}) = \frac{i}{\rho_{\alpha}} \lim_{\mathbf{p} \to 0} (\mathbf{D}_{\mathbf{k}_{\alpha}^{0}m} \cdot \boldsymbol{\nabla}_{\mathbf{p}}) e^{-i\mathbf{p} \cdot \boldsymbol{\rho}_{\alpha}}, \tag{82}$$

with

$$\mathbf{D}_{\mathbf{k}_{\alpha}^{0}m} = \epsilon_{\alpha\beta} e_{\alpha} (\lambda_{\beta} e_{\gamma} - \lambda_{\gamma} e_{\beta}) \int d\mathbf{r}_{\alpha} \psi_{\mathbf{k}_{\alpha}^{0}}^{(+)*}(\mathbf{r}_{\alpha}) \mathbf{r}_{\alpha} \psi_{\alpha m}(\mathbf{r}_{\alpha}), \tag{83}$$

and similarly for $D_{m\mathbf{k}_{\alpha}^{0}}(\hat{\boldsymbol{\rho}}_{\alpha})$ and $\mathbf{D}_{m\mathbf{k}_{\alpha}^{0}}$ (cf. (52)). Then we obtain from (81)

$$\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{\approx} \lim_{\mathbf{p},\mathbf{p}\to 0} \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \frac{(\mathbf{D}_{m\mathbf{k}_{\alpha}^{0}}\cdot\boldsymbol{\nabla}_{\mathbf{p}'})(\mathbf{D}_{\mathbf{k}_{\alpha}^{0}m}\cdot\boldsymbol{\nabla}_{\mathbf{p}})J(\mathbf{u})}{[E+i0-q_{\alpha}^{2}/2M_{\alpha}-k_{\alpha}^{0\,2}/2\mu_{\alpha}]}.$$
(84)

The integral $J(\mathbf{u})$ is given by (67). Making use of its asymptotic form (B.3) for $u \to 0$ we find

$$\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{=} C_m^{(c)}\Delta_{\alpha} + o\,(\Delta_{\alpha}),\tag{85}$$

with

$$C_m^{(c)} = -\frac{\pi^2}{4} \int \frac{d\mathbf{k}_{\alpha}^0}{(2\pi)^3} \frac{\left[|\mathbf{D}_{\mathbf{k}_{\alpha}^0 m}|^2 + |\hat{\mathbf{\Delta}}_{\alpha} \cdot \mathbf{D}_{\mathbf{k}_{\alpha}^0 m}|^2 \right]}{[E + i0 - q_{\alpha}^2/2M_{\alpha} - k_{\alpha}^{0^2}/2\mu_{\alpha}]}.$$
(86)

As in (68), we omitted also in (85) a Δ_{α} -independent term. We point out that from the discussion in the Appendix A follows that the result (85) with (86) is valid also for $q_{\alpha} = \sqrt{2M_{\alpha}E}$ where, in contrast to appearance, $C_m^{(c)}$ in (86) is not singular.

For on-shell scattering $(q'_{\alpha} = q_{\alpha} = \bar{q}_{\alpha})$, taking into account (78) the expression (86) simplifies to

$$C_{m}^{(c)} = \frac{\pi^{2}}{4} \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \frac{\left[|\mathbf{D}_{\mathbf{k}_{\alpha}^{0}m}|^{2} + |\hat{\boldsymbol{\Delta}}_{\alpha} \cdot \mathbf{D}_{\mathbf{k}_{\alpha}^{0}m}|^{2} \right]}{\left[|\hat{E}_{\alpha m}| + k_{\alpha}^{0\,2}/2\mu_{\alpha} \right]}.$$
(87)

That is, in the leading order $\mathcal{V}_{\alpha m,\alpha m(c)}^{opt\,(as)}$ depends neither on the incoming nor the outgoing momenta \mathbf{q}_{α} and \mathbf{q}_{α}' alone but only on the momentum transfer $\boldsymbol{\Delta}_{\alpha}$. It is also independent of the energy. Hence we can write (81) as

$$\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E_{\alpha m}+i0) \equiv \mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\boldsymbol{\Delta}_{\alpha})$$

$$\stackrel{\Delta_{\alpha}\to 0}{\approx} \int_{\boldsymbol{\rho}_{\alpha}\geq A} d\boldsymbol{\rho}_{\alpha} e^{-i\boldsymbol{\Delta}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} \mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\boldsymbol{\rho}_{\alpha}), \qquad (88)$$

where the local potential

$$\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\boldsymbol{\rho}_{\alpha}) = \left\{ \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \frac{|D_{\mathbf{k}_{\alpha}^{0}m}(\hat{\boldsymbol{\rho}}_{\alpha})|^{2}}{[|\hat{E}_{\alpha m}| + k_{\alpha}^{0\,2}/2\mu_{\alpha}]} \right\} \frac{1}{\rho_{\alpha}^{4}} \tag{89}$$

describes the coordinate-space asymptotics of $\mathcal{V}_{\alpha m,\alpha m(c)}^{opt(as)}$. It is the contribution to the polarisation potential from the intermediate three-body continuum states.

Summing up the contribution (68) with (69) from the intermediate two-fragment states and the contribution (85) with (86) from the intermediate three-particle continuum states, we thus have off the energy shell the final result

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{=} C_{1}\Delta_{\alpha} + o\,(\Delta_{\alpha}),\tag{90}$$

with

$$C_{1} = C_{m}^{(b)} + C_{m}^{(c)}$$

$$= -\frac{\pi^{2}}{4} \left\{ \sum_{n \neq m} \frac{\left[|\mathbf{D}_{nm}|^{2} + |\hat{\mathbf{\Delta}}_{\alpha} \cdot \mathbf{D}_{nm}|^{2} \right]}{[E + i0 - q_{\alpha}^{2}/2M_{\alpha} - \hat{E}_{\alpha n}]} + \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \frac{\left[|\mathbf{D}_{\mathbf{k}_{\alpha}^{0}m}|^{2} + |\hat{\mathbf{\Delta}}_{\alpha} \cdot \mathbf{D}_{\mathbf{k}_{\alpha}^{0}m}|^{2} \right]}{[E + i0 - q_{\alpha}^{2}/2M_{\alpha} - \hat{E}_{\alpha n}]} \right\}.$$
(91)

Consequently, for off-shell scattering we have found for the asymptotic behavior of the total optical potential (17), i.e. including the contribution from the static potential (for a spherically symmetric target state m), in the limit $\Delta_{\alpha} \to 0$ the result

$$\mathcal{V}_{\alpha m,\alpha m}^{opt}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{=} \frac{4\pi e_{\alpha}(e_{\beta}+e_{\gamma})}{\Delta_{\alpha}^{2}} + C_{1}\Delta_{\alpha} + o\left(\Delta_{\alpha}\right),\tag{92}$$

with the energy- and momentum-dependent factor $C_1 = C_1(q_{\alpha}, E)$ given by (91). It should be noted that the strength factor C_1 of the leading term decreases with increasing energy.

Equation (92) with (91) constitutes our first main result. It implies the exact compensation in the (non-static part of the) optical potential of the singular terms proportional to Δ_{α}^{-1} and $\ln \Delta_{\alpha}$, in contrast to their appearence (as discussed in [20] for negative energies) in the effective potentials which occur in the effective-two-body formulation of the three-charged particle theory. We emphasize that this compensation was proved here both on and off the energy shell, and for arbitrary total three-body energy E < 0 and E > 0. It generalizes the cancellation proofs, given in [18–23] for energies below the dissociation threshold, to positive energies. In addition, at negative three-particle energy our derivation avoids the various inconsistencies existing there.

If we consider on-shell scattering then, as follows from (68), (71), (85) and (87), $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}$ depends on the momenta only in the form of the momentum transfer Δ_{α} , and no longer on the energy, i.e.,

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E_{\alpha m}) \equiv \mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(\boldsymbol{\Delta}_{\alpha}).$$
(93)

Consequently, the inverse Fourier transform of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(\Delta_{\alpha})$ is a local, energy-independent potential describing the asymptotic behavior of the (non-static part of the) optical potential in coordinate space. From (73) and (89) we read off

$$\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(\boldsymbol{\rho}_{\alpha}) \stackrel{\rho_{\alpha} \to \infty}{=} -\frac{a}{2\rho_{\alpha}^{4}} + o\left(\frac{1}{\rho_{\alpha}^{4}}\right),\tag{94}$$

with

$$a = 2 \sum_{n \neq m} \frac{|D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha})|^2}{|\hat{E}_{\alpha m}| - |\hat{E}_{\alpha n}|} + 2 \int \frac{d\mathbf{k}_{\alpha}^0}{(2\pi)^3} \frac{|D_{\mathbf{k}_{\alpha}^0 m}(\hat{\boldsymbol{\rho}}_{\alpha})|^2}{|\hat{E}_{\alpha m}| + k_{\alpha}^{0^2}/2\mu_{\alpha}}.$$
(95)

As can be seen, the strength factor governing the coordinate-space behavior is just the static dipole polarisability as known from the perturbative approaches. That is, no remormalization of a arises from summing up all the higher order terms in the perturbation expansion of the full three-particle Green function G(z). Furthermore, all dependence on the incoming energy has disappeared (in contrast to the approximate result of ref. [17], but in agreement with the result obtained in [15] within the adiabatic approach).

For the coordinate-space behavior of the total optical potential, i.e. the inverse Fourier transform of (17), we derive on the energy shell for spherically symmetric targets

$$\mathcal{V}_{\alpha m,\alpha m}^{opt}(\boldsymbol{\rho}_{\alpha}) \stackrel{\rho_{\alpha} \longrightarrow \infty}{=} \frac{e_{\alpha}(e_{\beta} + e_{\gamma})}{\rho_{\alpha}} - \frac{a}{2\rho_{\alpha}^{4}} + o\left(\frac{1}{\rho_{\alpha}^{4}}\right).$$
(96)

Equation (96) with (95) is our second main result. It states that in the asymptotic expansion of the energy-shell restriction of the optical potential for large intercluster separation there occurs as the first nonvanishing term after the center-of-mass Coulomb interaction, which arises from the multipole expansion of the folded Coulomb channel interaction, the local (induced) polarisation potential $-a/2\rho_{\alpha}^4$. This result extends the one derived in [18–23] for E < 0, to arbitrary energies.

Simultaneously we derived the exact expression for the static dipole polarisability a. To our best knowledge this is the first derivation of a within the framework of a genuinly three-body, non-perturbative, non-adiabatic approach. In this context we point out that the same expression for a was derived in [18] for E < 0. However, in that derivation a spectral decomposition of the three-body Green function in $\Omega_{\alpha} \cap \Omega'_{\alpha}$ was used, which is inadequate since it does not take into account the long-ranged three-body correlations described in [24]. The latter necessarily lead to the appearence of the wave functions $\psi_{\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha})$ instead of $\psi_{\mathbf{k}_{\alpha}}^{(+)}(\mathbf{r}_{\alpha})$. Though, this inconsistency in [18] did not influence the final result. Nevertheless, we feel that it is important to present a consistent three-body derivation of the dipole polarisability.

IV. SUMMARY

We have investigated the singularity structure in momentum space of the optical potential responsible for the elastic scattering of a charged particle α off a bound state of two charged (or one charged and one neutral) particles, on the basis of the rigourous three-body scattering theory. Without having recourse to perturbative or other approximate methods we have shown that (for spherically symmetric bound states) the optical potential behaves, in the limit that the momentum transfer Δ_{α} goes to zero, as $C_0 \Delta_{\alpha}^{-2} + C_1 \Delta_{\alpha} + o(\Delta_{\alpha})$, for both negative and positive energies. That is, terms $\sim \Delta_{\alpha}^{-1}$ or $\sim \ln \Delta_{\alpha}$ cancel exactly. The factors appearing in this expansion have the familiar physical interpretation: C_0 is the product of the total charges of the colliding fragments, and C_1 is the general, energy- and momentum-dependent expression for the polarisability of the composite particle.

For on-shell scattering we find that this momentum-transfer behavior entails in coordinate space a local tail of the optical potential of the form $C_0/\rho_{\alpha} - a/2\rho_{\alpha}^4 + o(\rho_{\alpha}^{-4})$, where ρ_{α} denotes the distance of the elementary from the center of mass of the composite particle. The polarisability *a* derived here coincides with the expression as extracted in perturbative or similar approximate approaches. These results imply that

(i) the exact cancellation of terms $\sim \rho_{\alpha}^{-2}$ and $\sim \rho_{\alpha}^{-3}$ takes place for energies below and above the dissociation threshold,

(ii) no renormalization of the polarisability a due to summing up the infinite perturbation series occurs, and

(iii) the strength factor a which governs the long-distance behavior in coordinate space is independent of the incident energy (in contrast to its off-shell analog C_1 which determines the strength of the corresponding singularity in momentum space).

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APPENDIX A:

In this Appendix we first investigate the behavior in the limit $\Delta_{\alpha} \equiv |\mathbf{q}'_{\alpha} - \mathbf{q}_{\alpha}| \to 0$ of the contribution of the *n*-th intermediate bound state in expression (57), to be denoted by $\mathcal{V}^{opt\,(as)}_{\alpha m,\alpha m\,(n)}$, at the discrete point $q_{\alpha} = q_{\alpha n}$. To simplify the considerations we replace the Coulomb scattering wave functions $\psi^{(+)*}_{\mathbf{q}^{\alpha}_{\alpha}}(\boldsymbol{\rho}_{\alpha})$ and $\psi^{(+)}_{\mathbf{q}^{\alpha}_{\alpha}}(\boldsymbol{\rho}'_{\alpha})$ by their leading terms for large distances, namely by the planes waves $e^{-i\mathbf{q}^{0}_{\alpha}}\cdot\boldsymbol{\rho}_{\alpha}$ and $e^{i\mathbf{q}^{0}_{\alpha}}\cdot\boldsymbol{\rho}'_{\alpha}$, respectively. We also omit the functions $D_{nm}(\hat{\boldsymbol{\rho}}_{\alpha})$ and $D_{mn}(\hat{\boldsymbol{\rho}}'_{\alpha})$. By doing so the question of the integrability or non-integrability of the singularities under considerations is not influenced. We therefore consider

$$\mathcal{V}_{\alpha m,\alpha m(n)}^{opt(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to0}{\sim} 2M_{\alpha} \lim_{\delta\to+0} \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \int_{\rho_{\alpha}\geq A} d\rho_{\alpha} \frac{\int_{\rho_{\alpha}\geq A} d\rho_{\alpha} \frac{e^{i(\mathbf{q}_{\alpha}^{0}-\mathbf{q}_{\alpha}')\cdot\boldsymbol{\rho}_{\alpha}'}}{\rho_{\alpha}'^{2}}}{\rho_{\alpha}'^{2}} \\
\times e^{-\delta\rho_{\alpha}'} \frac{1}{[q_{\alpha n}^{2}+i0-q_{\alpha}^{0}]^{2}}e^{-\delta\rho_{\alpha}} \frac{-e^{i(\mathbf{q}_{\alpha}^{0}-\mathbf{q}_{\alpha})\cdot\boldsymbol{\rho}_{\alpha}}}{\rho_{\alpha}^{2}}}{\rho_{\alpha}^{2}} \\
\stackrel{\Delta_{\alpha}\to0}{\sim} \lim_{\delta\to+0} \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \frac{1}{\sqrt{(\mathbf{q}_{\alpha}^{0}-\mathbf{q}_{\alpha}')^{2}+\delta^{2}}} \frac{1}{[q_{\alpha n}^{2}+i0-q_{\alpha}^{0}]^{2}}}{\lambda_{\alpha}'^{2}} \\
\times \frac{1}{\sqrt{(\mathbf{q}_{\alpha}^{0}-\mathbf{q}_{\alpha})^{2}+\delta^{2}}}.$$
(A.1)

The integrals over ρ_{α} and ρ'_{α} from 0 to A added in the second line are certainly less singular than the original expression; hence they do not alter our conclusion. We use the integral representation

$$\frac{1}{\sqrt{\zeta}} = \frac{1}{2\pi} \oint d\beta \frac{1}{\sqrt{\beta}} \frac{1}{\beta + \zeta} = \frac{1}{\pi} \int_0^\infty d\beta \frac{1}{\sqrt{\beta}} \frac{1}{\beta + \zeta},\tag{A.2}$$

where \oint means the integral along a closed contour around the point $\beta = -\zeta$; in the integral from 0 to ∞ of the second representation we must have $\arg \beta = 0$. This leads to

$$\mathcal{V}_{\alpha m,\alpha m(n)}^{opt(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{\sim} \lim_{\delta\to+0} \int_{0}^{\infty} d\beta \frac{1}{\sqrt{\beta}} \int_{0}^{\infty} d\alpha \frac{1}{\sqrt{\alpha}} J(\beta,\alpha;\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha},q_{\alpha n}), \tag{A.3}$$

with

$$J(\beta, \alpha; \mathbf{q}'_{\alpha}, \mathbf{q}_{\alpha}, q_{\alpha n}) = \int \frac{d\mathbf{q}^{0}_{\alpha}}{(2\pi)^{3}} \frac{1}{[\beta + (\mathbf{q}^{0}_{\alpha} - \mathbf{q}'_{\alpha})^{2} + \delta^{2}]} \frac{1}{[q^{2}_{\alpha n} + i0 - q^{0}_{\alpha}]^{2}} \frac{1}{[\alpha + (\mathbf{q}^{0}_{\alpha} - \mathbf{q}_{\alpha})^{2} + \delta^{2}]}.$$
 (A.4)

This integral is explicitly known [29],

$$J(\beta, \alpha; \mathbf{q}'_{\alpha}, \mathbf{q}_{\alpha}, q_{\alpha n}) = -\frac{1}{8\pi} \frac{1}{\sqrt{c^2 - ab}} \ln\left[\frac{c + \sqrt{c^2 - ab}}{c - \sqrt{c^2 - ab}}\right],\tag{A.5}$$

with

$$ab = [\Delta_{\alpha}^{2} + (\sqrt{\alpha} + \sqrt{\beta})^{2}][q_{\alpha}^{2} + (\sqrt{\alpha} - iq_{\alpha n})^{2}][q_{\alpha}^{'2} + (\sqrt{\beta} - iq_{\alpha n})^{2}],$$
(A.6)

$$c = -iq_{\alpha n}[\Delta_{\alpha}^{2} + (\sqrt{\alpha} + \sqrt{\beta})^{2}] + \sqrt{\beta}[q_{\alpha}^{2} + \alpha - q_{\alpha n}^{2}] + \sqrt{\alpha}[q_{\alpha}^{'2} + \beta - q_{\alpha n}^{2}].$$
(A.7)

Because of the presence of the parameters α and β , the regularisation parameter δ is no longer needed. We therefore have already put δ equal to zero in (A.5) - (A.7). For $q_{\alpha} = q'_{\alpha} = q_{\alpha n}$, (A.6) and (A.7) simplify to

$$ab = \sqrt{\alpha}\sqrt{\beta} [\Delta_{\alpha}^{2} + (\sqrt{\alpha} + \sqrt{\beta})^{2}] [\sqrt{\alpha} - 2iq_{\alpha n}] [\sqrt{\beta} - 2iq_{\alpha n}], \qquad (A.8)$$

$$c = -iq_{\alpha n} [\Delta_{\alpha}^{2} + (\sqrt{\alpha} + \sqrt{\beta})^{2}] + \sqrt{\alpha \beta} [\sqrt{\alpha} + \sqrt{\beta}].$$
(A.9)

Substitution of $\alpha = \Delta_{\alpha}^2 v$ and $\beta = \Delta_{\alpha}^2 t$ in (A.8) and (A.9) shows that in the limit $\Delta_{\alpha} \to 0$

$$ab \sim \Delta_{\alpha}^4, \quad c \sim \Delta_{\alpha}^2, \quad \text{i.e., } \sqrt{c^2 - ab} \sim \Delta_{\alpha}^2.$$
 (A.10)

Introducing (A.5) into (A.3), changing to the new variables v and t, and taking into account (A.10), it is immediately seen that the main term of $\mathcal{V}_{\alpha m,\alpha m(n)}^{opt\,(as)}$ is independent of Δ_{α} in the limit $\Delta_{\alpha} \to 0$ at the discrete point $q_{\alpha} = q_{\alpha n}$, i.e., it is regular there. Hence the same holds true also for the sum over all intermediate bound state contributions $\mathcal{V}_{\alpha m,\alpha m(b)}^{opt\,(as)}$.

The other problem concerns the behavior of the intermediate three-body continuum part (74) if $q_{\alpha} = q_{\alpha 1}$, where $q_{\alpha 1} = \sqrt{2M_{\alpha}E}$. In that case we are not a priori allowed to take out the propagator $d_{k_{\alpha}^{0}}(q_{\alpha}^{0})$ from under the integral over \mathbf{q}_{α}^{0} at the point $q_{\alpha}^{0} = q_{\alpha}$. To investigate this case consider the definition (75) of $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$. Since in the limit $\Delta_{\alpha} \to 0$ the leading, Δ_{α} -dependent term is defined by $\boldsymbol{\rho}_{\alpha} \approx \boldsymbol{\rho}_{\alpha}'$, the exponential Coulomb distorsion factors cancel. That is, it suffices to consider

$$L(\mathbf{q}_{\alpha}^{0};\boldsymbol{\rho}_{\alpha},\boldsymbol{\rho}_{\alpha}') \approx \int \frac{d\mathbf{k}_{\alpha}^{0}}{(2\pi)^{3}} \frac{D_{m\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha}')(\hat{\boldsymbol{\rho}}_{\alpha}')D_{\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})m(\hat{\boldsymbol{\rho}}_{\alpha})}{[E+i0-q_{\alpha}^{0^{2}}/2M_{\alpha}-k_{\alpha}^{0^{2}}/2\mu_{\alpha}]}.$$
(A.11)

If we perform the \mathbf{k}_{α}^{0} -integration, the pole of $d_{k_{\alpha}^{0}}(q_{\alpha}^{0})$ can give rise to a singularity of $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ in the q_{α}^{0} -plane at $q_{\alpha}^{0} = q_{\alpha 1}$. It is an end point singularity which arises from the coincidence of the propagator pole at $k_{\alpha}^{0} = \sqrt{\mu_{\alpha}(q_{\alpha 1}^{2} - q_{\alpha}^{0})/M_{\alpha}}$ with the lower limit $k_{\alpha}^{0} = 0$ of integration over k_{α}^{0} . Since the leading, Δ_{α} -dependent term of $\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}$ in the limit $\Delta_{\alpha} \to 0$ is generated by the coincidence of the singularities of the integrand in the integral (74) over \mathbf{q}_{α}^{0} at the point $\mathbf{q}_{\alpha}^{0} = \mathbf{q}_{\alpha} = \mathbf{q}_{\alpha}'$, the appearence of an additional singularity, namely in the the function L, will influence the leading term of $\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}$.

To investigate the analytic behavior of $L(\mathbf{q}^0_{\alpha}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}'_{\alpha})$ for $q^0_{\alpha} - q_{\alpha 1} \to 0$, consider the integrand in (A.11). The denominator has a zero that can cause the singularity under consideration. The behavior for $k^0_{\alpha} \to 0$ of the numerator (cf. (51)) is defined by the wave function $\psi^{(+)}_{\mathbf{k}^0_{\alpha}}(\boldsymbol{\rho}_{\alpha})(\mathbf{r}_{\alpha})$ which we write as

$$\psi_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha}) = \exp\left[\frac{\mathbf{a}_{\alpha}(\hat{\boldsymbol{\rho}}_{\alpha})}{\rho_{\alpha}} \cdot \boldsymbol{\nabla}_{\mathbf{k}_{\alpha}^{0}}\right]\psi_{\mathbf{k}_{\alpha}^{0}}^{(+)}(\mathbf{r}_{\alpha})$$
$$\approx \psi_{\mathbf{k}_{\alpha}^{0}}^{(+)}(\mathbf{r}_{\alpha}) + \frac{\mathbf{a}_{\alpha}(\hat{\boldsymbol{\rho}}_{\alpha}) \cdot \boldsymbol{\nabla}_{\mathbf{k}_{\alpha}^{0}}}{\rho_{\alpha}}\psi_{\mathbf{k}_{\alpha}^{0}}^{(+)}(\mathbf{r}_{\alpha}) + O\left(\frac{1}{\rho_{\alpha}^{2}}\right).$$
(A.12)

The threshold behavior for $k_{\alpha}^{0} \to 0$ of the scattering wave function $\psi_{\mathbf{k}_{\alpha}^{0}}^{(+)}(\mathbf{r}_{\alpha})$ in the potential $V_{\alpha} = V_{\alpha}^{S} + V_{\alpha}^{C}$ is entirely given by the corresponding behavior of the Coulomb scattering wave function $\psi_{C,\mathbf{k}_{\alpha}^{0}}^{(+)}(\mathbf{r}_{\alpha})$. This follows from the wellknown fact that the threshold behavior of the radial wave functions for two charged particles is the same for all the partial waves and is defined by the factor [30]

$$|N_{\alpha}| = \left[\frac{2\pi\eta_{\alpha}^{0}}{e^{2\pi\eta_{\alpha}^{0}} - 1}\right]^{\frac{1}{2}}.$$
 (A.13)

Therefore, the behavior of the full wave function $\psi_{\mathbf{k}_{\alpha}^{0}}^{(+)}(\mathbf{r}_{\alpha})$ for $k_{\alpha}^{0} \to 0$ is governed by the same factor, and the one of the numerator in (A.11) by $|N_{\alpha}|^{2}$.

Hence we have to distinguish two cases.

1. The Coulomb potential V_{α}^{C} is repulsive, i.e., $\eta_{\alpha}^{0} > 0$. Then for $k_{\alpha}^{0} \to 0$ one has $|N_{\alpha}|^{2} \approx 2\pi \eta_{\alpha}^{0} e^{-2\pi \eta_{\alpha}^{0}} \to 0$. The exponential smallness of the numerator for $k_{\alpha}^{0} \to 0$ compensates any zero of the denominator at the point $k_{\alpha}^{0} = 0$. In other words, the pole of the propagator in (A.11) at $k_{\alpha}^{0} = \sqrt{\mu_{\alpha}(q_{\alpha 1}^{2} - q_{\alpha}^{0})/M_{\alpha}}$ does not generate a singularity of $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ at the point $q_{\alpha}^{0} = q_{\alpha 1}$. Thus, when extracting the leading term of $\mathcal{V}_{\alpha m,\alpha m}^{opt\,(as)}(c)$ for $\Delta_{\alpha} \to 0$, the function $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ can be taken out from under the integral over \mathbf{q}_{α}^{0} at the point $\mathbf{q}_{\alpha}^{0} = \mathbf{q}_{\alpha}$, as in the case $q_{\alpha} \neq q_{\alpha 1}$. The consequence is that the behavior of the optical potential is the same for all q_{α} including $q_{\alpha} = q_{\alpha 1}$, namely $\sim O(\Delta_{\alpha})$.

2. The Coulomb potential V_{α}^{C} is attractive, i.e., $\eta_{\alpha}^{0} < 0$. In this case, $|N_{\alpha}|^{2} \approx 2\pi \eta_{\alpha}^{0} \rightarrow \infty$ for $k_{\alpha}^{0} \rightarrow 0$, and hence all terms in the expansion (A.12) become singular. This difficulty can be overcome as follows. According [24] the wave function $\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$, as given by (37), is asymptotic solution of the three-particle Schrödinger equation in the region Ω_{α} , i.e., it satisfies this equation up to terms $O(1/\rho_{\alpha}^{2})$ (cf. (43)). From the derivation given there it is, however, easily seen that for $k_{\alpha}^{0} = 0$, taking into account the local momentum $\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})$ in the asymptotic solution $\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}^{(+)as}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$ instead of its asymptotic value $\mathbf{k}_{\alpha}^{0} = 0$, gives corrections $\sim O(1/\rho_{\alpha}^{2})$ to the Schrödinger equation in Ω_{α} . Therefore, in a small vicinity of $k_{\alpha}^{0} = 0$ the asymptotic solution $\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$ may be replaced by the function $\psi_{\mathbf{k}_{\alpha}^{(+)}}^{(+)as}(\boldsymbol{\rho}_{\alpha})$ in $\psi_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})e^{i\eta_{\alpha}^{0}ln(k_{\beta}^{0}\boldsymbol{\rho}_{\alpha}-\epsilon_{\alpha\beta}\mathbf{k}_{\beta}^{0}\cdot\boldsymbol{\rho}_{\alpha})e^{i\eta_{\alpha}^{0}ln(k_{\alpha}^{0}\boldsymbol{\rho}_{\alpha}-\epsilon_{\alpha\gamma}\mathbf{k}_{\alpha}^{0}\cdot\boldsymbol{\rho}_{\alpha})$, i.e., by (37) but with \mathbf{k}_{α}^{0} substituting $\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})$ in $\psi_{\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha})(\mathbf{r}_{\alpha})$. Hence for arbitrary k_{α}^{0} we may rewrite the asymptotic solution $\Psi_{\mathbf{q}_{\alpha}^{0}\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha},\mathbf{r}_{\alpha})$ in the form (37) with

$$\mathbf{k}_{\alpha}^{0}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha}^{0} + \chi(k_{\alpha}^{0}) \frac{\mathbf{a}_{\alpha}(\hat{\boldsymbol{\rho}}_{\alpha})}{\rho_{\alpha}}, \qquad (A.14)$$

where $\chi(k_{\alpha}^{0})$ is a characteristic function, which equals one everywhere except for a small neighbourhood of $k_{\alpha}^{0} = 0$, and goes smoothly to zero when k_{α}^{0} approaches zero. Thus, taking into account the factor $k_{\alpha}^{0^{2}}$ from the phase volume, the behavior of the numerator in (A.11) in the limit $k_{\alpha}^{0} \to 0$ is governed by $k_{\alpha}^{0^{2}} |N_{\alpha}|^{2} \sim k_{\alpha}^{0}$.

Let us write $L(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ as the sum $L = L_{\varepsilon} + \tilde{L}_{\varepsilon}$, where L_{ε} denotes the integral over \mathbf{k}_{α}^{0} over the interior of a small sphere with radius ε . \tilde{L}_{ε} contains the remaining integral. Since the latter does not contain the origin $k_{\alpha}^{0} = 0$, $\tilde{L}_{\varepsilon}(\mathbf{q}_{\alpha}^{0}; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$ is regular at $q_{\alpha}^{0} = q_{\alpha 1} = q_{\alpha}$ and can therefore be taken out from under the integral over \mathbf{q}_{α}^{0} in (74) at the point $\mathbf{q}_{\alpha}^{0} = \mathbf{q}_{\alpha}$. The consequence is that at the momentum $q_{\alpha} = q_{\alpha 1}$, its contribution to the optical potential V_{α}^{C} is $\sim O(\Delta_{\alpha})$, i.e. of the same order as for $q_{\alpha} \neq q_{\alpha 1}$.

However, $L_{\varepsilon}(\mathbf{q}_{\alpha}^{0};\boldsymbol{\rho}_{\alpha},\boldsymbol{\rho}_{\alpha}')$ is singular at $q_{\alpha}^{0} = q_{\alpha 1}$. When performing the \mathbf{k}_{α}^{0} -integration, the pole of $d_{k_{\alpha}^{0}}(q_{\alpha}^{0})$ gives rise to a behavior $L_{\varepsilon}(\mathbf{q}_{\alpha}^{0};\boldsymbol{\rho}_{\alpha},\boldsymbol{\rho}_{\alpha}') \sim \ln(q_{\alpha}^{0\,2}+i0-q_{\alpha 1}^{2})$ in the q_{α}^{0} -plane. In order to arrive at this result we singled out from the product $D_{m\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha}')(\hat{\boldsymbol{\rho}}_{\alpha}')D_{\mathbf{k}_{\alpha}^{0}}(\boldsymbol{\rho}_{\alpha})m(\hat{\boldsymbol{\rho}}_{\alpha})$ the factor $|N_{\alpha}|^{2}$ which is singular at $k_{\alpha}^{0} = 0$, and ignored the rest since it remains finite. Denote by $\mathcal{V}_{\alpha m,\alpha m(\varepsilon)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E)$ that part of $\mathcal{V}_{\alpha m,\alpha m(c)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E)$ which contains $L_{\varepsilon}(\mathbf{q}_{\alpha}^{0};\boldsymbol{\rho}_{\alpha},\boldsymbol{\rho}_{\alpha}')$ instead of $L(\mathbf{q}_{\alpha}^{0};\boldsymbol{\rho}_{\alpha},\boldsymbol{\rho}_{\alpha}')$ (cf. (74)). Substituting $\ln(q_{\alpha}^{0^2} + i0 - q_{\alpha 1}^2)$ for $L_{\varepsilon}(\mathbf{q}_{\alpha}^0; \boldsymbol{\rho}_{\alpha}, \boldsymbol{\rho}_{\alpha}')$, and integrating over $\boldsymbol{\rho}_{\alpha}$ and $\boldsymbol{\rho}_{\alpha}'$, gives

$$\mathcal{V}_{\alpha m,\alpha m\,(\varepsilon)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E) \stackrel{\Delta_{\alpha}\to 0}{\sim} \lim_{\delta\to+0} \int \frac{d\mathbf{q}_{\alpha}^{0}}{(2\pi)^{3}} \frac{\ln\left(q_{\alpha 1}^{2}+i0-q_{\alpha}^{0}\right)^{2}}{\sqrt{(\mathbf{q}_{\alpha}^{0}-\mathbf{q}_{\alpha}')^{2}+\delta^{2}}\sqrt{(\mathbf{q}_{\alpha}^{0}-\mathbf{q}_{\alpha})^{2}+\delta^{2}}}.$$
 (A.15)

When writing down this expression we already took into account that the behavior of $\mathcal{V}_{\alpha m,\alpha m\,(\varepsilon)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E)$ for $\Delta_{\alpha} \to 0$ is defined by the region $\boldsymbol{\rho}_{\alpha} \approx \boldsymbol{\rho}_{\alpha}'$ where the product of the Coulomb distortion factors equals one. The integration region over \mathbf{q}_{α}^{0} in (A.15) supposedly consists only of the neighbourhood of $\mathbf{q}_{\alpha}^{0} \approx \mathbf{q}_{\alpha} \approx \mathbf{q}_{\alpha}'$. Comparing with (A.1) (putting there $q_{\alpha n}$ equal to $q_{\alpha 1}$) we conclude that expression (A.15) is less singular at $\Delta_{\alpha} \to 0$ than (A.1). Hence, in the case of an attractive Coulomb potential V_{α}^{C} , for $q_{\alpha} = q_{\alpha 1}$ the contribution $\mathcal{V}_{\alpha m,\alpha m\,(\varepsilon)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E)$, and thus also $\mathcal{V}_{\alpha m,\alpha m\,(c)}^{opt\,(as)}(\mathbf{q}_{\alpha}',\mathbf{q}_{\alpha};E)$, is finite in the limit $\Delta_{\alpha} \to 0$.

APPENDIX B:

In this Appendix we evaluate the integral (67) and extract its asymptotic behavior for $u \to 0$. Substituting the new variable $v = u\rho_{\alpha}$ and making use of eqs. 3.761(2) and 8.352(3) of [31] we obtain

$$J(u) = 2\pi i u^{3} [\Gamma(-4, i u A) - \Gamma(-4, -i u A)] =$$

= $\frac{i\pi u^{3}}{12} [\Gamma(0, i u A) - \Gamma(0, -i u A)] - \sum_{m=0}^{3} \frac{m!}{(i u A)^{m+1}} \left(e^{i u A} + (-1)^{m} e^{-i u A} \right), \quad (B.1)$

where $\Gamma(\mu, x)$ is the incomplete Gamma function [31]. With the help of eqs. 3.761(2), 8.230(1) and 8.232(1) of [31] one finds

$$\Gamma(0, iuA) - \Gamma(0, -iuA) = 2i\operatorname{si}(uA) = -i\pi + \sum_{m=0}^{\infty} \frac{(-1)^{m+1}(uA)^{2m-1}}{(2m-1)(2m-1)!},$$
(B.2)

where si(x) is the sine-integral. Substitution of (B.2) into (B.1) leads to the following asymptotic behavior of J(u) for $u \to 0$:

$$J(u) \stackrel{u \to 0}{=} \frac{4\pi}{3A^3} - \frac{2\pi}{3A}u^2 + \frac{\pi^2}{12}u^3 + O(u^4).$$
(B.3)

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