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Reactions with three charged particles in final state

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Abstract. Three-particle Coulomb asymptotic states are derived. The knock-out reaction amplitude with distorted waves in the initial and final states is extracted using the Faddeev equations. The conditions are discussed under which this amplitude can be approximated by the distorted wave impulse amplitude. The influence of the Coulomb final state interaction on the differential quasielastic knock-out cross section is investigated. To this end the main singular part of the DWIA amplitude is singled out and compared with conventional approximations. The application of the present results to the $(e, 2e)$ reactions will be done in the next paper.

1. Introduction

We shall consider the reaction

$$1+(23) \rightarrow 1+2+3 \tag{1}$$

where (23) is the neutral bound state of particles 2 and 3; particles 1, 2, 3 are non-identical, spinless charged particles. In principle, the rigorous theory of these processes, within the framework of the three-body problem based on the solution of the Faddeev differential equations, is developed by Merkurjev (1981). However, the calculations in Merkurjev's approach have not yet been undertaken because of the computational difficulties. It is, therefore, of interest to find simple methods for calculating the reaction (1) amplitude such that the main characteristics of the process could be taken into account.

Specifically, we are interested in quasielastic knock-out reactions with charged particles, in particular, the $(e, 2e)$ process. To calculate these reactions, the formalism of the distorted wave impulse approximation (DWIA) has been used (McCarthy and Weigold 1976). In this paper we attempt the derivation of the reaction (1) amplitude with distorted waves in the initial and final states (DWA) within the framework of the three-body problem. Using the Faddeev equations we extracted the DWA amplitude M_{DWA} from the exact amplitude. This amplitude is represented as an infinite series, every term of which corresponds to the definite mechanism. The first term of the series is the usual DWIA amplitude M_{DWIA}. For the pure Coulomb interactions between particles 1, 2 and 3 M_{DWA} may be approximated by NM_{DWIA} where N is the renormalisation factor, whose appearance is due to the influence of mechanisms more complicated than the impulse approximation.

The calculations are performed in different approximations because of the computational difficulties. These include the factorised DWIA (Dixon *et al* 1978) and the eikonal approximation (Ugbabe *et al* 1975). In as much as reaction (1) yields three charged

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particles, the purely Coulomb part of the interaction strongly affects the process characteristics at low incident energies. In this case, different approximations require due care because of the long-range character of the Coulomb interaction. Therefore, taking the *ee*-scattering off-shell amplitude outside the integral defining the matrix element (as is done in the factorised DWIA for $(e, 2e)$ reactions) can distort the final result, but this, however, is disguised by the distortion effects calculated in the optical model. It will also be noted that the correct inclusion of the Coulomb interaction in the eikonal approximation is not a simple task. For example, the papers Dixon *et al* (1978) and Stefani and Camilloni (1978) suggest the eikonal approximation wherein the distorted waves are replaced by the equation

$$\chi_{\boldsymbol{k}}^{(+)}(\boldsymbol{r})=\exp(-\gamma kR)\exp[\mathrm{i}(1+\beta+\mathrm{i}\gamma)\boldsymbol{kr}] \tag{2}$$

where γ, β and R are the adjusting parameters. This approximation is valid for the initial distorted wave, describing the scattering of electrons by an atom. However, for the final distorted waves describing the electron scattering by ions, such an approximation is not valid since it is well known (Merkurjev 1977) that the main term of $\chi_{\boldsymbol{k}}^{(+)}(\boldsymbol{r})$ at $r\to\infty(\boldsymbol{kr}\neq kr)$ is given by the Coulomb distorted plane wave, $\exp[\mathrm{i}kr-\mathrm{i}\eta\ln(kr-\boldsymbol{kr})]$ where η is the Coulomb parameter which cannot be approximated by equation (2).

This paper is devoted to the investigation of the influence of the final state Coulomb interaction on the angular dependence and the absolute value of the quasielastic knock-out differential cross section. We have neglected the distortions in the initial and final state due to the polarisation interactions (i.e. interactions which are decreasing at large distances more rapidly than the Coulomb one). These polarisation interactions can be included in the calculation, for example, in the eikonal approximation, as was done by Stefani and Camilloni (1978).

Without solving the Faddeev–Merkurjev equations, we extract the main singular term of the reaction amplitude in an explicit form near the quasielastic peak which will be helpful in calculating the quasielastic knock-out cross section and, also, in studying the accuracy of different approximations used in atomic physics to take into account the Coulomb effects. The formulae obtained in what follows can be used for arbitrary charged particles. The results of calculations for the $(e, 2e)$ reactions will be given in the next paper.

2. Three-particle Coulomb asymptotic states

We first consider the two-particle Coulomb scattering. In van Haeringen (1976) the scattering theory of two charged particles is developed using the so-called Coulomb asymptotic states (CAS) which are the generalisations of the usual asymptotic states (δ-functions in the momentum space or plane waves in the coordinate space) for the case of charged particles. In the momentum representation the CAS is determined by the relation

$$\langle\boldsymbol{p}\,|\,\boldsymbol{k}\infty\rangle=8\pi\exp(-\tfrac{1}{2}\pi\eta)\Gamma(2+\mathrm{i}\eta)\lim_{\delta\to+0}\frac{[p^2-(k+\mathrm{i}\delta)^2]^{\mathrm{i}\eta}}{[(\boldsymbol{p}-\boldsymbol{k})^2+\delta^2]^{2+\mathrm{i}\eta}}. \tag{3}$$

Here $\eta=Z_1Z_2\mu/k$ is the Coulomb parameter, k and μ are the relative momentum and reduced mass of the interacting particles. At $\eta=0$ $\langle\boldsymbol{p}\,|\,\boldsymbol{k}\infty\rangle=(2\pi)^3\delta(\boldsymbol{p}-\boldsymbol{k})$. In what follows it will be seen that the most singular term of the Fourier transform of the Coulomb distorted plane wave is, in fact, the CAS $\langle\boldsymbol{p}\,|\,\boldsymbol{k}\infty\rangle$. The main term of the distorted plane wave in a non-singular direction ($\hat{k}\boldsymbol{r} \neq kr$) at $r \to \infty$ is given by the expression (Merkurjev 1977)

$$\chi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r}) = \exp[\mathrm{i}(\boldsymbol{kr} + W)], \qquad W = \eta \ln(kr - \boldsymbol{kr}). \tag{4}$$

Then the Fourier transform of $\chi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r})$ is

$$\chi_{\boldsymbol{k}}^{(0)}(\boldsymbol{p}) = -\lim_{\delta \to +0} \frac{\mathrm{d}}{\mathrm{d}\delta} \int \mathrm{d}\boldsymbol{r} \exp(-\mathrm{i}\boldsymbol{pr}) \frac{\exp(-\delta r)}{r} \chi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r})$$

$$= 8\pi \exp(\tfrac{1}{2}\pi\eta) \frac{1}{\Gamma(-\mathrm{i}\eta)} \lim_{\delta \to +0} \frac{[2(\boldsymbol{kq} + \mathrm{i}k\delta)]^{\mathrm{i}\eta}}{(q^2 + \delta^2)^{2+\mathrm{i}\eta}}$$

$$\times \int_0^\infty \mathrm{d}v\, v^{-1-\mathrm{i}\eta}(1+v)^{-2}\left[\delta + \mathrm{i}kv \frac{q^2 + \delta^2}{2(\boldsymbol{kq} + \mathrm{i}k\delta)}\right].$$

Here $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{p}$ and $2(\boldsymbol{kq} + \mathrm{i}k\delta) = (k + \mathrm{i}\delta)^2 - p^2 + q^2 + \delta^2$. The most singular term of $\chi_{\boldsymbol{k}}^{(0)}(\boldsymbol{p})$ at $q^2 + \delta^2 = 0$ is identical with $\langle \boldsymbol{p} | \boldsymbol{k}\infty \rangle$. Thus, $\chi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r})$ is the main term of the CAS in the coordinate representation at $r \to \infty$.

From this result we can now define the three-particle CAS. The main term of the three-particle distorted plane wave in a non-singular direction is given by the relation (in the CMS system) (Merkurjev 1977)

$$\chi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(0)}(R) = \exp[\mathrm{i}KR + W] \tag{5}$$

where

$$W = W_{12} + W_{13} + W_{23}, \qquad W_{\beta\gamma} = \eta_{\beta\gamma} \ln \xi_{\beta\gamma},$$

$$\eta_{\beta\gamma} = Z_\beta Z_\gamma \mu_{\beta\gamma} / k_{\beta\gamma}, \qquad \xi_{\beta\gamma} = k_{\beta\gamma} r_{\beta\gamma} - \boldsymbol{k}_{\beta\gamma} \boldsymbol{r}_{\beta\gamma},$$

$R = \{\boldsymbol{\rho}_\alpha, \boldsymbol{r}_{\beta\gamma}\}$ and $K = \{\boldsymbol{k}_\alpha, \boldsymbol{k}_{\beta\gamma}\}$ are vectors of the six-dimensional coordinate and momentum space, respectively; $\boldsymbol{r}_{\beta\gamma} = \boldsymbol{r}_\beta - \boldsymbol{r}_\gamma$, ρ_α is the radius vector connecting particle α and the centre of mass of the pair $\beta + \gamma$; $\boldsymbol{k}_{\beta\gamma} = (m_\gamma \boldsymbol{k}_\beta - m_\beta \boldsymbol{k}_\gamma)/m_{\beta\gamma}$ is the relative momentum of particles β and γ; $m_{\beta\gamma} = m_\beta + m_\gamma$; $\boldsymbol{r}_\beta$, $\boldsymbol{k}_\beta$, m_β are the radius-vector, momentum and the mass of particle β, respectively. The Fourier transforms of $\chi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(0)}(R)$ is the convolution of the Fourier transforms of $\chi_{\boldsymbol{k}_{\beta\gamma}}^{(0)}$:

$$\chi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(0)}(\boldsymbol{p}_1, \boldsymbol{p}_2) = \int \mathrm{d}\boldsymbol{p}(2\pi)^{-3} \chi_{\boldsymbol{k}_{12}}^{(0)}(\boldsymbol{p}) \chi_{\boldsymbol{k}_{13}}^{(0)}(\boldsymbol{p}_1 - \boldsymbol{k}_1 - \boldsymbol{p} + \boldsymbol{k}_{12} + \boldsymbol{k}_{13})$$

$$\times \chi_{\boldsymbol{k}_{23}}^{(0)}(\boldsymbol{p}_2 - \boldsymbol{k}_2 + \boldsymbol{p} - \boldsymbol{k}_{12} + \boldsymbol{k}_{23}). \tag{6}$$

Replacing each function $\chi_{\boldsymbol{k}_{\beta\gamma}}^{(0)}(\boldsymbol{p}_{\beta\gamma})$ in equation (6) by the corresponding main singular term, i.e. by CAS $\langle \boldsymbol{p}_{\beta\gamma} | \boldsymbol{k}_{\beta\gamma}\infty \rangle$ we arrive at the expression for the three-particle CAS:

$$\langle P | K\infty \rangle \equiv \langle \boldsymbol{p}_1, \boldsymbol{p}_2 | \boldsymbol{k}_1, \boldsymbol{k}_2\infty \rangle$$

$$= \int \mathrm{d}\boldsymbol{p}(2\pi)^{-3} \langle \boldsymbol{p} | \boldsymbol{k}\infty \rangle \langle \boldsymbol{p}_1 - \boldsymbol{k}_1 - \boldsymbol{p} + \boldsymbol{k}_{12} + \boldsymbol{k}_{13} | \boldsymbol{k}_{13}\infty \rangle$$

$$\times \langle \boldsymbol{p}_2 - \boldsymbol{k}_2 + \boldsymbol{p} - \boldsymbol{k}_{12} + \boldsymbol{k}_{23} | \boldsymbol{k}_{23}\infty \rangle,$$

$$\boldsymbol{p}_1 + \boldsymbol{p}_2 + \boldsymbol{p}_3 = 0, \qquad \boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_2 = 0. \tag{7}$$

It can be seen that

$$\int \mathrm{d}\boldsymbol{p}_1(2\pi)^{-3}\, \mathrm{d}\boldsymbol{p}_2(2\pi)^{-3} f(\boldsymbol{p}_1, \boldsymbol{p}_2) d(\boldsymbol{p}_1, \boldsymbol{p}_2) \langle \boldsymbol{p}_1, \boldsymbol{p}_2 | \boldsymbol{k}_1, \boldsymbol{k}_2\infty \rangle = f(\boldsymbol{k}_1, \boldsymbol{k}_2), \tag{8}$$

$$d(p_1, p_2) = (\mathscr{E} - E - \mathrm{i}\delta)^{\mathrm{i}\eta}(m_{12}/4k_{12}^2)^{\mathrm{i}\eta_{12}}(m_{13}/4k_{13}^2)^{\mathrm{i}\eta_{13}} \times (m_{23}/4k_{23}^2)^{\mathrm{i}\eta_{23}}\, \mathrm{e}^{-\pi\eta/2}\Gamma(1-\mathrm{i}\eta) \tag{9}$$

where $f(P) = f(\boldsymbol{p}_1, \boldsymbol{p}_2)$ is a regular function at $\boldsymbol{p}_1 = \boldsymbol{k}_1$ and $\boldsymbol{p}_2 = \boldsymbol{k}_2$ and $f(P) \in \mathscr{L}_\infty(R^6)$; $P = \{\{\boldsymbol{p}_3, \boldsymbol{p}_{12}\}$, $\mathscr{E} = p_3^2/2\mu_3 + p_{12}^2/2\mu_{12}$, $E = k_3^2/2\mu_3 + E_{12}$ is the total three-particle energy, $E_{ij} = k_{ij}^2/2\mu_{ij}$, $\eta = \eta_{12} + \eta_{13} + \eta_{23}$, $\mu_3 = m_3 m_{12}/M$, $M = m_1 + m_2 + m_3$. We have omitted here the cumbersome proof of equation (8). It will be noted that in derivation of this relation one should take into account that the two-particle CAS's in equation (7) have their own infinitesimal $\delta \to +0$. The expression (8) implies that on the class of the functions $f(P)(\mathscr{E} - E - \mathrm{i}\delta)^{\mathrm{i}\eta}$, $\delta \to +0$, where $f(P)$ is a regular function at the point $P = K$, the three-particle CAS acts as

$$\langle P|K\infty\rangle = (2\pi)^6\delta(P-K)d^{-1}(p_1, p_2), \tag{10}$$

$\delta(P-K)$ is the δ-function in the six-dimensional momentum space.

It should be noted that the expression (10) coincides with the asymptotic state obtained by Komarov *et al* (1983) within the framework of non-stationary formalism. However, equation (10) is valid only on the class of the functions $f(P)(\mathscr{E} - E - \mathrm{i}\delta)^{\mathrm{i}\eta}$ where equations (7) and (10) are equivalent, however, in the general case the expression (7) must be used for the three-body CAS.

3. Quasielastic knock-out amplitude with three charged particles in the final state for infinitely heavy particle 3

3.1.

The reaction amplitude can be written as

$$M = \langle\Psi^{(-)}|U_{23}|\Phi_i\rangle. \tag{11}$$

Here $U_{\alpha\beta} = V - V_{\alpha\beta}$, $V = V_{12} + V_{13} + V_{23}$, $V_{\alpha\beta}$ is the interaction potential of particles α and β, that is, in general, the sum of Coulomb and polarisation potentials,

$$\Phi_i = \exp(\mathrm{i}\boldsymbol{k}_i\boldsymbol{\rho}_1)\varphi_{23}(\boldsymbol{r}_{23}), \tag{12}$$

$\boldsymbol{k}_i$ is the relative momentum of colliding particles, φ_{23} is the bound state (23) wavefunction. The three-particle wavefunction $\Psi^{(-)}$ describing the scattering of three charged particles can be written as

$$\Psi^{(-)} = \Psi^{(12)(-)} + G^{(-)}V_{12}\Psi^{(12)(-)}, \tag{13}$$

where $\Psi^{(12)(-)}$ is the three-particle wavefunction neglecting the interaction of particles 1 and 2,

$$G^{(\pm)} = (E - H_0 - V \pm \mathrm{i}\delta)^{-1}, \qquad \delta \to +0,$$

H_0 is the operator of the total three-particle kinetic energy. The wavefunction $\Psi^{(12)(\pm)}$ satisfies the equation

$$\Psi^{(12)(\pm)}_{\boldsymbol{k}_1,\boldsymbol{k}_2} = |\boldsymbol{k}_1, \boldsymbol{k}_2\infty\pm\rangle + (E - H_0 \pm \mathrm{i}\delta)^{-1}U_{12}\Psi^{(12)(\pm)}_{\boldsymbol{k}_1,\boldsymbol{k}_2}, \tag{14}$$

$$|\boldsymbol{k}_1, \boldsymbol{k}_2\infty+\rangle \equiv |\boldsymbol{k}_1, \boldsymbol{k}_2\infty\rangle, \qquad |\boldsymbol{k}_1, \boldsymbol{k}_2\infty-\rangle = |\boldsymbol{k}_1, \boldsymbol{k}_2\infty+\rangle^*.$$

Note that in equation (14) the inhomogeneous term is the three-particle CAS which is defined by equation (7) in the impulse representation. In the coordinate representation this CAS is the Coulomb distorted plane wave.

Now substituting (13) into (11) provides

$$M=\langle\Psi^{(12)(-)}|V_{13}|\Phi_i\rangle+\langle\Psi^{(12)(-)}|V_{12}|\Psi_i^{(+)}\rangle, \tag{15}$$

where

$$\Psi_i^{(+)}=\Phi_i+G^{(+)}U_{23}\Phi_i$$

is the wavefunction describing the collision of incident particle 1 with bound state (23). When $m_{1,2}\ll m_3$ (for example, in the reaction $(e,2e)$) the terms $\sim m_{1,2}/m_3$ can be neglected. Then the solution of equation (14) can be written down in the impulse representation as

$$\Psi^{(12)(\pm)}_{k_1,k_2}(p_1,p_2)=\int \mathrm{d}p(2\pi)^{-3}\Psi^{(\pm)}_{k_1}(p_1-p+k_{12})\Psi^{(\pm)}_{k_2}(p_2+p-k_{12})\langle p|k_{12}\infty\pm\rangle, \tag{16}$$

$\Psi_k^{(\pm)}(p)$ is the Coulomb wavefunction in the impulse representation. If we insert this equation into equation (15) then, by virtue of orthogonality of discrete and continuum wavefunctions of particle 2 in the field of infinitely heavy particle 3, the first term in equation (15) will be equal to zero and

$$M=\langle\Psi^{(12)(-)}|V_{12}|\Psi_i^{(+)}\rangle. \tag{17}$$

This expression for M including equation (16) is the generalisation of the known formula for the knock-out reaction amplitude (in post-form) with infinitely heavy particle 3 (Baz *et al* 1971) to the case of three charged particles in the final state.

3.2.

From the Faddeev equations for $\Psi_i^{(+)}$ we single out the elastic component $\Psi_{i,\mathrm{el}}^{(+)}$ describing the elastic scattering of particle 1 from the bound state (23). This enables us to extract from the amplitude M the term with distorted waves in the initial and final states in an explicit form. At $m_3=\infty$ the Faddeev equations are reduced to two equations (Baz *et al* (1971)) which can be recorded as

$$\Psi_{23}^{(+)}=\Phi_i+G_{23}^{(+)}V_{23}\hat{\Psi}_{23}^{(+)}, \qquad \hat{\Psi}_{23}^{(+)}=\hat{G}_{23}^{(+)}U_{23}\Psi_{23}^{(+)} \tag{18a, b}$$

where

$$\Psi_i^{(+)}=\Psi_{23}^{(+)}+\hat{\Psi}_{23}^{(+)}, \qquad G_{\beta\gamma}^{(+)}=(E-H_0-V_{\beta\gamma}+\mathrm{i}\delta)^{-1},$$
$$\hat{G}_{\beta\gamma}^{(+)}=(E-H_0-U_{\beta\gamma}+\mathrm{i}\delta)^{-1}, \qquad G_0^{(+)}=(E-H_0+\mathrm{i}\delta)^{-1}, \qquad \delta\to+0. \tag{19}$$

It should be noted that for charged particles the differential Faddeev–Merkurjev equations (Merkurjev 1981) must be used. These equations are not solved here yet, they are used to rearrange equation (18). Therefore, we can use the usual Faddeev equations (18) on the assumption that all Coulomb potentials are screened. Nevertheless, the final result is valid for unscreened Coulomb potentials as well.

From equation (18) and (19) we obtain

$$\Psi_i^{(+)}=\hat{G}_{23}^{(+)}V_{23}\Phi_i+\hat{G}_{23}^{(+)}T_{23}\hat{\Psi}_{23}^{(+)}, \tag{20}$$

where

$$\Phi_i=G_0^{(+)}V_{23}\Phi_i, \qquad \hat{G}_{23}^{(+)}=G_0^{(+)}+\hat{G}_{23}^{(+)}U_{23}G_0^{(+)}, \qquad G_{23}^{(+)}V_{23}=G_0^{(+)}T_{23}.$$

Here, $T_{\beta\gamma}$ is the scattering operator of particles β and γ in the three-particle space.

For T_{23} the spectral decomposition can be written as

$$T_{23}=V_{23}|\varphi_{23}\rangle g_1\langle\varphi_{23}|V_{23}+\sum_n V_{23}|\varphi_{23}^{(n)}\rangle g_1^{(n)}\langle\varphi_{23}^{(n)}|V_{23}+\tilde{T}_{23}, \tag{21}$$

$$g_1^{(n)}=(E+\varepsilon_{23}^{(n)}-H_1+\mathrm{i}\delta)^{-1},$$

H_1 is the operator of relative kinetic energy of particle 1 and the centre of mass of (23), $\varepsilon_{23}^{(n)}$ is the binding energy of the nth bound state of (23). For the ground state $\varepsilon_{23}^{(0)}\equiv\varepsilon_{23}$,

$$\varphi_{23}^{(0)}\equiv\varphi_{23} \qquad \text{and} \qquad g_1^{(0)}\equiv g_1=(E+\varepsilon_{23}-H_1+\mathrm{i}\delta)^{-1}.$$

It should be noted that

$$\langle\boldsymbol{k}'|g_1^{(n)}|\boldsymbol{k}\rangle=(2\pi)^3\delta(\boldsymbol{k}'-\boldsymbol{k})\left(E_1^{(n)}-\frac{k_1^2}{2\mu_1}+\mathrm{i}\delta\right)^{-1},$$

$$E_1^{(n)}=E+\varepsilon_{23}^{(n)}, \qquad \mu_1=m_1m_{23}/M.$$

In equation (21) the first term is the contribution to T_{23} from the pole corresponding to the ground bound state of (23); the sum Σ_n contains the contributions from other poles corresponding to the excited bound states of (23); $\tilde{T}_{23}$ includes the contributions from the Born term V_{23} and the continuum.

It is easy to see that

$$T(\boldsymbol{k},\boldsymbol{k}_i)=\langle\boldsymbol{k},\varphi_{23}|V_{23}|\hat{\Psi}_{23}^{(+)}\rangle=\langle\boldsymbol{k},\varphi_{23}|V_{23}\hat{G}_{23}^{(+)}U_{23}|\Psi_{23}^{(+)}\rangle \tag{22}$$

and

$$T^{(n)}(\boldsymbol{k},\boldsymbol{k}_i)=\langle\boldsymbol{k},\varphi_{23}^{(n)}|V_{23}\hat{G}_{23}^{(+)}U_{23}|\Psi_{23}^{(+)}\rangle \tag{23}$$

are the half-shell amplitudes of the elastic and inelastic scattering of particle 1 on (23). Substituting equation (20) into (17) and taking into account equations (22) and (23) provides

$$M=M_0+\sum_n M_n+\tilde{M}, \tag{24}$$

$$M_0=\langle\Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)}|V_{12}\hat{G}_{23}V_{23}|\Psi_{\boldsymbol{k}_i,\mathrm{el}}^{(+)}\rangle, \tag{25}$$

$$M_n=\int \mathrm{d}\boldsymbol{k}(2\pi)^{-3}\langle\Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)}|V_{12}\hat{G}_{23}^{(+)}V_{23}|\varphi_{23}^{(n)},\boldsymbol{k}\rangle(E_1^{(n)}-k^2/2\mu_1+\mathrm{i}\delta)^{-1}T^{(n)}(\boldsymbol{k},\boldsymbol{k}_i), \tag{26}$$

$$\tilde{M}=\langle\Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)}|V_{12}\hat{G}_{23}^{(+)}\tilde{T}_{23}|\hat{\Psi}_{23}^{(+)}\rangle. \tag{27}$$

Here

$$\Psi_{\boldsymbol{k}_i,\mathrm{el}}^{(+)}=\Phi_{\boldsymbol{k}_i}^{(+)}\varphi_{23} \tag{28}$$

is the elastic component of $\Psi_i^{(+)}$. In the momentum representation

$$\Phi_{\boldsymbol{k}_i}^{(+)}(\boldsymbol{k})=(2\pi)^3\delta(\boldsymbol{k}_i-\boldsymbol{k})+\frac{T(\boldsymbol{k}_i,\boldsymbol{k})}{E_1-k^2/2\mu_1+\mathrm{i}\delta}.$$

In the numerical calculations $\Phi_{\boldsymbol{k}_i}^{(+)}$ can be approximated by the optical wavefunction $\chi_{\boldsymbol{k}_i}^{(+)}$. In this case M_0 is converted to the DWA amplitude

$$M_{\mathrm{DWA}}=\langle\Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)}|V_{12}\hat{G}_{23}^{(+)}V_{23}|\varphi_{23},\chi_{\boldsymbol{k}_i}^{(+)}\rangle. \tag{29}$$

Thus, from the exact amplitude M we extracted the DWA amplitude containing the distorted waves in the initial and final states. The reaction mechanism in the DWA, i.e. the reaction amplitude in the plane wave approximation, is given by the expression

$$B = \langle \boldsymbol{k}_1, \boldsymbol{k}_2 | V_{12} \hat{G}_{23}^{(+)} V_{23} | \varphi_{23}, \boldsymbol{k}_i \rangle. \tag{30}$$

This amplitude can be represented as a sum of the infinite series of non-relativistic Feynman graphs (see figure 1). Each graph of this series corresponds to the definite member of the expansion.

$$V_{12}\hat{G}_{23}^{(+)} = T_{12}G_0^{(+)} + T_{12}G_0^{(+)}T_{13}G_0^{(+)} + T_{12}G_0^{(+)}T_{13}G_0^{(+)}T_{12}G_0^{(+)} + \ldots . \tag{31}$$

As can be seen from equation (31) and figure 1 the amplitude M_{DWA} contains the contributions from all possible rescatterings of particle 1 from particles 2 and 3 after knock-out of particle 2. The first member in M_{DWA} is the DWIA (distorted wave impulse approximation) amplitude M_{DWIA}. Thus the extracted amplitude M_{DWA} is not identical to M_{DWIA}. As opposed to the DWIA, the DWA is based on the three-particle dynamics. From the results of the work (Mukhamedzhanov 1982) it can be shown that for the purely Coulomb potentials inclusion of all Coulomb scatterings of particle 1 from particles 2 and 3 leads to the simple renormalisation of the amplitude M_{DWIA}, i.e. the main term of M_{DWA} can be written in the form

$$\begin{aligned} M_{\mathrm{DWA}}^{(S)} &= N M_{\mathrm{DWIA}}, \\ M_{\mathrm{DWIA}} &= \langle \Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)} | T_{12} G_0^{(+)} V_{23} | \varphi_{23}, \chi_{\boldsymbol{k}_i}^{(+)} \rangle. \end{aligned} \tag{32}$$

We have omitted here the formula for N, which will be given in the next publication. The main terms of M_n and $\tilde{M}$ for the purely Coulomb potentials $V_{\beta\gamma}$ are given by the expressions

$$M_n^{(s)} = N_n M_{n,\mathrm{DWIA}},$$

$$M_{n,\mathrm{DWIA}} = \int \mathrm{d}\boldsymbol{k} (2\pi)^{-3} \langle \Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)} | T_{12} G_0^{(+)} V_{23} | \varphi_{23}^{(n)}, \boldsymbol{k} \rangle \, (E_i^{(n)} - k^2/2\mu_1 + \mathrm{i}\delta)^{-1} T^{(n)}(\boldsymbol{k}, \boldsymbol{k}_i), \tag{33}$$

$$\tilde{M}^{(s)} = \tilde{N} \tilde{M}_{\mathrm{DWIA}}, \tag{34}$$

$$\tilde{M}_{\mathrm{DWIA}} = \int \mathrm{d}\boldsymbol{k} (2\pi)^{-3} \langle \Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)} | T_{12} G_0^{(+)} \tilde{T}_{23} | \hat{\Psi}_{23}^{(+)} \rangle. \tag{35}$$

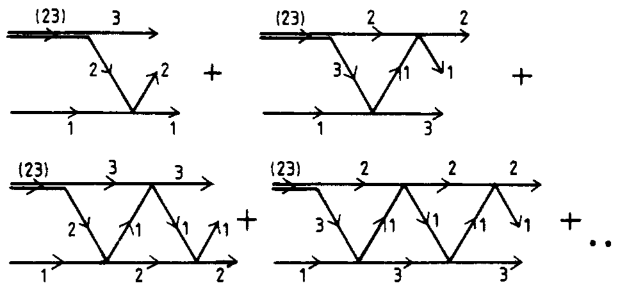

Figure 1. The reaction amplitude in the plane wave approximation represented as a sum of the infinite series of non-relativistic Feynman graphs.

Thus the main term of the quasielastic knock-out reaction amplitude for the pure Coulomb potentials $V_{\beta\gamma}$ is then

$$M^{(s)} = M_0^{(s)} + \sum_n M_n^{(s)} + \tilde{M}^{(s)}. \tag{36}$$

Equation (36) is one of the main results of this work. For the $(e, 2e)$ reaction on atoms at high incident energies ($E_i \gg \varepsilon_{23}$) the inelastic scattering amplitudes can be calculated on the Born approximation. Since these amplitudes are negligible at high energies the amplitudes $M_n^{(s)}$ and $\tilde{M}^{(s)}$ are small as compared with M_{DWA} near the quasielastic peak. Besides at high energies $|N| \approx 1$ and the reaction amplitude M near the quasielastic peak can be well approximated by M_{DWIA} (equation (32)). The concrete calculations for the $(e, 2e)$ reaction will be given in the next paper.

3.3.

Our primary purpose in this work is to study the influence of the Coulomb scattering in the final state upon the amplitude M_{DWIA} in the region of the quasielastic peak that is described by the wavefunction $\Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)}$. In what follows all the potentials $V_{\beta\gamma}$ will, therefore, be regarded as the purely Coulomb ones. Let us consider equation (32) and extract its main term near the quasielastic peak resulting from the nearby singularity of the reaction amplitude in the σ-plane at $\sigma = q^2 + \varkappa_{23}^2 = 0$, $q^2 = (\boldsymbol{k}_i - \boldsymbol{k}_1 - \boldsymbol{k}_2)^2$, $\varkappa_{23}^2 = 2\mu_{23}\varepsilon_{23}$ (Avakov *et al* 1972). Therefore, the most singular part of M_{DWIA} at $\sigma = 0$ provides the main contribution to the quasielastic peak and the extraction of the main term of M_{DWIA} is equivalent to the extraction of the most singular part of M_{DWIA}.

Consider equation (32) in the momentum representation. Since our interest is to study the influence of the Coulomb final-state rescattering we replace the initial distorted wave $\chi_{\boldsymbol{k}_i}^{(+)}$ by the plane wave $|\boldsymbol{k}_i\rangle$. As was noted the polarisation effects can be included using the eikonal approximation. Then for M_{DWIA} we get

$$M_{\mathrm{DWIA}}(\boldsymbol{k}_i; \boldsymbol{k}_1, \boldsymbol{k}_2) = \int \frac{\mathrm{d}\boldsymbol{p}_1}{(2\pi)^3} \frac{\mathrm{d}\boldsymbol{p}_2}{(2\pi)^3} \Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(+)}(\boldsymbol{p}_1, \boldsymbol{p}_2) t_{12}(\boldsymbol{p}_{12}, \boldsymbol{q}_{12}; E_{12}) \varphi_{23}(\boldsymbol{q}_{23}), \tag{37}$$

where we used

$$T_{12}(\boldsymbol{p}_3', \boldsymbol{p}_{12}; \boldsymbol{p}_3, \boldsymbol{q}_{12}; E_{12}) = (2\pi)^3 \delta(\boldsymbol{p}_3' - \boldsymbol{p}_3) t_{12}(\boldsymbol{p}_{12}, \boldsymbol{q}_{12}; E_{12})$$

and t_{12} is the half-shell amplitudes of the Coulomb scattering of particles 1 and 2; $\boldsymbol{q}_{12} = \boldsymbol{k}_i - (m_1/m_{12})(\boldsymbol{p}_1 + \boldsymbol{p}_2)$, $\boldsymbol{p}_{12} = (m_2\boldsymbol{p}_1 - m_1\boldsymbol{p}_2)/m_{12}$ are the relative momenta of particles 1 and 2 before and after scattering, respectively; $E_{12} = k_{12}^2/2\mu_{12}$, $\boldsymbol{q}_{23} = \boldsymbol{k}_i - \boldsymbol{p}_1 - \boldsymbol{p}_2$ is the momentum of particles 2 in the bound state (23), $\boldsymbol{k}_i$ is the momentum of the incident particle 1. Besides, it was taken into account that $[\Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(-)}(\boldsymbol{p}_1, \boldsymbol{p}_2)]^* = \Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(+)}(\boldsymbol{p}_1, \boldsymbol{p}_2)$.

The singularity of the integral (37) at $\sigma = 0$ results from the coincidence of the singularity of the function $t_{12}(\boldsymbol{p}_{12}, \boldsymbol{q}_{12}; E_{12})\varphi_{23}(\boldsymbol{q}_{23})$ at

$$\sigma_{23} = q_{23}^2 + \varkappa_{23}^2 = 0 \tag{38}$$

with the singularities of the wavefunction $\Psi_{\boldsymbol{k}_1,\boldsymbol{k}_2}^{(12)(+)}(\boldsymbol{p}_1, \boldsymbol{p}_2)$ at $\boldsymbol{p}_1 = \boldsymbol{k}_1$ and $\boldsymbol{p}_2 = \boldsymbol{k}_2$. The wavefunction $\varphi_{23}(\boldsymbol{q}_{23})$ can be written as (Blokhintsev *et al* 1977):

$$\varphi_{23}(\boldsymbol{q}_{23}) = \tilde{W}(\boldsymbol{q}_{23})/\sigma_{23}^{1-\eta_0} \tag{39}$$

where $\eta_0 = Z_2 Z_3 m_2/\varkappa_{23}$ is the Coulomb parameter of particle 2 in the bound state (23), $\tilde{W}(\boldsymbol{q}_{23})$ is the reduced vertex form factor which is regular at $\sigma_{23}=0$. At $\sigma_{23}=0$ $q_{12}^2 = k_{12}^2$, i.e. $\sigma_{23}=0$ is the singular point of t_{12}. At $q_{12} \to k_{12}$ we have (Dolinsky and Mukhamedzhanov 1966, van Haeringen 1976)

$$t_{12}(\boldsymbol{p}_{12}, \boldsymbol{q}_{12}; E_{12}) \underset{q_{12}\to k_{12}}{\approx} -2\exp(-\pi\eta_{12})k_{12}\eta_{12}|\Gamma(1+\mathrm{i}\eta_{12})|^2 \frac{(\tilde{\sigma}\sigma')^{\mathrm{i}\kappa_{12}}}{(2k_{12})^{2\mathrm{i}\eta_{12}}(q_{1i})^{2+2\mathrm{i}\eta_{12}}}, \tag{40}$$

$\tilde{\sigma} = (\mu_{12}/m_2)\sigma_{23} = q_{12}^2 - k_{12}^2 - \mathrm{i}\delta$, $\sigma' = p_{12}^2 - \kappa_{12}^2 - \mathrm{i}\delta$, $\boldsymbol{q}_{1i} = \boldsymbol{k}_1 - \boldsymbol{k}_i$. If we insert relations (39) and (40) into equation (37) and take outside the integral sign all the factors that are regular at $\sigma_{23}=0$ and $\sigma'=0$ at points $\boldsymbol{p}_1 = \boldsymbol{k}_1$ and $\boldsymbol{p}_2 = \boldsymbol{k}_2$, then at or near the singularity $\sigma = 0$

$$M_{\mathrm{DWIA}} \approx -2\exp(-\pi\eta_{12})k_{12}\eta_{12}|\Gamma(1+\mathrm{i}\eta_{12})|^2\left(\frac{\mu_{12}}{m_2}\right)^{\mathrm{i}\eta_{12}}(2k_{12})^{-2\mathrm{i}\eta_{12}}(q_{i1})^{-2-2\mathrm{i}\eta_{12}}W_{23}(\boldsymbol{q})J, \tag{41}$$

$$J = \int \frac{\mathrm{d}\boldsymbol{p}_1}{(2\pi)^3}\frac{\mathrm{d}\boldsymbol{p}_2}{(2\pi)^3}\frac{(\sigma')^{\mathrm{i}\eta_{12}}}{\sigma_{23}^{1-\eta_0-\mathrm{i}\eta_{12}}}\Psi^{(+)}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{p}_1, \boldsymbol{p}_2). \tag{42}$$

In order to extract the most singular part of M_{DWIA} at $\sigma = 0$ we must substitute equation (16) into equation (42) and perform the integration over $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ and, then, over $\boldsymbol{p}$. When the main term of J is separated out from the integrals over $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ the factor $(\sigma')^{\mathrm{i}\eta_{12}}$ can be taken outside the integral sign at points $\boldsymbol{p}_1 = \boldsymbol{k}_1 + \boldsymbol{p} - \boldsymbol{k}_{12}$ and $\boldsymbol{p}_2 = \boldsymbol{k}_2 - \boldsymbol{p} + \boldsymbol{k}_{12}$ which are the singular points of the Coulomb wavefunctions $\Psi^{(+)}_{\boldsymbol{k}_1}(\boldsymbol{p}_1 - \boldsymbol{p} + \boldsymbol{k}_{12})$ and $\Psi^{(+)}_{\boldsymbol{k}_2}(\boldsymbol{p}_2 + \boldsymbol{p} - \boldsymbol{k}_{12})$ (Guth and Mullin 1951), i.e. the factorisation provides

$$(\sigma')^{\mathrm{i}\eta_{12}} = (p^2 - k_{12}^2 - \mathrm{i}\boldsymbol{\delta})^{\mathrm{i}\eta_{12}}. \tag{43}$$

Consider now the integral over $\boldsymbol{p}_1$:

$$L_1 = \int \mathrm{d}\boldsymbol{p}_1 (2\pi)^{-3}\sigma_{23}^{-1+\eta_0+\mathrm{i}\eta_{12}}\Psi^{(+)}_{\boldsymbol{k}_1}(\boldsymbol{p}_1 - \boldsymbol{p} + \boldsymbol{k}_{12}). \tag{44}$$

From Cauchy's theorem

$$\sigma_{23}^{-\lambda} = \frac{1}{2\pi\mathrm{i}}\oint \mathrm{d}x \cdot x^{-\lambda}\frac{1}{x - \sigma_{23}} \tag{45}$$

where the integral over x is taken along a closed contour so that the singularity $x = \sigma_{23}$ is inside this contour. Substituting equation (45) into equation (44) we can calculate the integral over $\boldsymbol{p}_1$ by using the formula

$$\int \frac{\mathrm{d}\boldsymbol{p}_1}{(2\pi)^3}\frac{1}{(\boldsymbol{p}_1 - \boldsymbol{a})^2 + \alpha^2}\Psi^{(+)}_{\boldsymbol{k}_1}(\boldsymbol{p}_1) = \exp(-\pi\eta_1/2)\Gamma(1+\mathrm{i}\eta_1)\frac{[a^2 - (k_1 + \mathrm{i}\alpha)^2]^{\mathrm{i}\eta_1}}{[(\boldsymbol{k}_1 - \boldsymbol{a})^2 + \alpha^2]^{1+\mathrm{i}\eta_1}},$$

$\eta_\beta = Z_\beta Z_3 m_\beta / k_\beta$. This relation can be obtained by going over to the coordinate representation (Guth and Mullin 1951). Inserting the expression obtained into the integral over x one can easily separate the main term of the integral over x. The integral over $\boldsymbol{p}_2$ is calculated in complete analogy with the integral over $\boldsymbol{p}_1$. Then the final expression for the main term at $\sigma \to 0$ of the reaction amplitude in the Coulomb distorted wave impulse approximation is

$$M^{(s)}_{\mathrm{DWIA}}(\boldsymbol{k}_i; \boldsymbol{k}_1, \boldsymbol{k}_2)$$
$$= -2\left(\frac{m_2}{\mu_{12}}\right)^{-\mathrm{i}\eta_{12}} \frac{k_{12}\eta_{12}\Gamma(1+\mathrm{i}\eta_{12})}{(\boldsymbol{k}_i-\boldsymbol{k}_1)^{2+2\mathrm{i}\eta_{12}}} \exp[-\tfrac{1}{2}\pi(\eta_1+\eta_2+\eta_{12})]$$
$$\times \frac{\Gamma[1-\eta_0+\mathrm{i}(\eta_1+\eta_2-\eta_{12})]}{\Gamma(1-\eta_0-\mathrm{i}\eta_{12})} \varphi_{23}(\boldsymbol{q})[(\boldsymbol{k}_2-\boldsymbol{k}_i)^2-(k_1+\mathrm{i}\varkappa_{23})^2]^{\mathrm{i}\eta_1}$$
$$\times[(\boldsymbol{k}_1-\boldsymbol{k}_i)^2-(k_2+\mathrm{i}\varkappa_{23})^2]^{\mathrm{i}\eta_2}\sigma^{-\mathrm{i}(\eta_1+\eta_2-\eta_{12})}. \tag{47}$$

Thus, by virtue of equation (39) at $\sigma \to 0$

$$M_{\mathrm{DWIA}}(\boldsymbol{k}_i; \boldsymbol{k}_1, \boldsymbol{k}_2) \sim \sigma^{-1+\eta_0-\mathrm{i}(\eta_1+\eta_2-\eta_{12})}. \tag{48}$$

Let us now discuss why it is important to have the correct knowledge of the true behaviour of the reaction amplitude at $\sigma \to 0$. In the dispersion approach (Avakov *et al* 1972) the quasielastic peak at $q^2=0$ is due to the presence of the nearby singularity at $\sigma=0$ in the reaction amplitude. The character of the singularity $\sigma=0$ of the amplitude M_{DWIA} is defined by equation (48). To compare the proximity of the singular point $\sigma=0$ to the point of the quasielastic peak $q^2=0$ it is convenient to introduce the dimensionless variable $z=\cos\sigma=-\boldsymbol{k}_3\boldsymbol{k}_i/k_3k_i$, where $\boldsymbol{k}_3=-\boldsymbol{k}_1-\boldsymbol{k}_2$. Then the point $z=1$ at the boundary of the physical region $(-1\leqslant z\leqslant 1)$ corresponds to the point $q^2=0$ and

$$z=\xi=\frac{k_i^2+k_3^2+\varkappa_{23}^2}{2k_ik_3}>1 \tag{49}$$

lying in the unphysical region corresponds to the singularity point $\sigma=0$. At quasielastic peak (with the neglect of the distortion effects)

$$\xi=1+(m_2/m_1)\varepsilon_{23}/E_{\mathrm{i}}. \tag{50}$$

For the $(e, 2e)$ processes at incident electron energies E_{i} of the order of several hundreds of eV $\xi\approx 1$. For example, for the $(e, 2e)$ reaction on He at $E_{\mathrm{i}}=400$ eV $\xi=1.03$. Hence, the singularity of the reaction amplitude at $z=\xi$ is in close proximity to the quasielastic peak. The main contribution to the reaction amplitude near the quasielastic peak is, therefore, provided by the main term at $\sigma=0 (z=\xi)$ which can be helpful in calculating the angular distribution and the absolute value of the differential cross section near the quasielastic peak.

The concrete calculations of the DWIA amplitude are performed in different approximations. The formula (47) enables one to estimate the accuracy of these approximations. For example, the main singular term of the factorised DWIA (FDWIA) (Dixon *et al* 1978) at $\sigma\to 0$ is related to $M^{(s)}_{\mathrm{DWIA}}$ as

$$M^{(s)}_{\mathrm{DWIA}}=D_{\mathrm{F}}M^{(s)}_{\mathrm{FDWIA}} \tag{51}$$

where

$$D_{\mathrm{F}}=\frac{\Gamma(1-\eta_0)}{\Gamma[1-\eta_0+\mathrm{i}(\eta_1+\eta_2)]}\,\frac{\Gamma[1-\eta_0+\mathrm{i}(\eta_1+\eta_2-\eta_{12})]}{\Gamma(1-\eta_0-\mathrm{i}\eta_{12})}. \tag{52}$$

Evidently, that the factor D_F can be used to determine an error in the absolute value of the FDWIA amplitude at the quasielastic peak.

For the Coulomb distorted wave Born approximation (CDWBA) (Namuri and Chen 1982)

$$M^{(s)}_{\rm DWIA} = D_{\rm C} M^{(s)}_{\rm CDWBA} \tag{53}$$

where

$$D_{\rm C} = [\Gamma(1 + i\eta_{12}) \exp(-\pi\eta_{12}/2)] D_{\rm F}/\sigma^{-i\eta_{12}}. \tag{54}$$

The results of calculations of the $(e, 2e)$ and (e^+, e^+e) reactions on atoms in the symmetric complanar kinematics will be given in the next paper.

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