

# Chapter 1

## Strong-Field S-Matrix Series with Coulomb Wave Final State

F.H.M. Faisal

**Abstract** Despite its long-standing usefulness for the analysis of various processes in intense laser fields, it is well-known that the KFR or strong-field approximation (SFA) does not account for the final-state Coulomb interaction for ionisation. Various *ad hoc* attempts have been made in the past to face this problem within the SFA, however, till now no systematic S-matrix expansion accounting for it has been found. To overcome this long standing limitation of SFA we present here a systematic series expansion of the strong-field S-matrix that could accounts for the final-state Coulomb interaction in all orders.

### 1.1 Introduction

Over the past several decades the well-known strong-field approximation in the form of the so-called KFR or SFA ansatz [1–3] has provided much fruitful insights into the highly non-perturbative processes in intense laser fields. However, it is also well-known that SFA does not account for the Coulomb interaction in the final state that is specially significant for the ubiquitous ionisation process in strong fields. Due to this problem, many authors in the past decades have made various *heuristic* corrections to the SFA. Thus, for example, attempts to account for the Coulomb effect appear within early ionisation models [4–6]. Other approaches include WKB-like approximations [7, 8], semi-classical and/or “quantum trajectory” approach [9–11], semi-analytic R-matrix approach [12], and more recently an approach employing ansätze with phase correction plus inhomogeneous differential equation [13]. Until now, however, no systematic strong-field S-matrix theory could be found that unlike the usual plane-wave SFA would be able to account for the laser plus Coulomb interaction in the final state to all orders.

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Here we present a strong-field S-matrix theory that overcomes this long standing problem and derive a *systematic* all order S-matrix series explicitly incorporating the laser plus Coulomb interaction in the final state. To this end we shall use below a three-interaction formalism developed earlier in connection with the so-called intense-field S-matrix theory or IMST (see, e.g. review [14] or, original references cited therein).

## 1.2 Three-Interaction Formalism

In this section we briefly indicate the three-interaction technique suitable for the problem at hand. The Schroedinger equation of the interacting atom+ laser field is

$$(i\hbar \frac{\partial}{\partial t} - H(t))|\Psi(t)\rangle = 0 \quad (1.1)$$

where  $H(t)$  is the total Hamiltonian of the system,

$$H(t) = H_a + V_i(t) \quad (1.2)$$

For example, for an effective one electron atomic system interacting with a laser field, we may take

$$H_a = (\frac{\mathbf{p}_{op}^2}{2m} - \frac{Ze^2}{r} + V_{s.r.}(\mathbf{r})) \quad (1.3)$$

where  $Z$  is the core charge and  $V_{s.r.}(\mathbf{r})$  is a short-range potential that goes to zero for asymptotically large  $r$  faster than the Coulomb potential.

The laser-atom interaction is assumed here in the minimal coupling gauge (in “dipole approximation”)

$$V_i(t) = (-\frac{e}{mc}\mathbf{A}(t) \cdot \mathbf{p}_{op} + \frac{e^2 A^2(t)}{2mc^2}) \quad (1.4)$$

where  $\mathbf{A}(t)$  is the vector potential of the laser field, and  $\mathbf{p}_{op} \equiv -i\hbar \nabla$ .

Since all information of the interacting system is contained in the full wavefunction  $\Psi(t)$  and in general this is not known explicitly, we shall consider a more useful formal expression of the full wavefunction in terms of the appropriate partial interactions among the sub-systems and, the associated sub-propagators (or Green’s functions). The latter objects may be already known, or could be found, to expand the total wavefunction in terms of them.

Thus, first, we may formally define the full propagator,  $G(t, t')$ , associated with the total Hamiltonian  $H(t)$ , by the inhomogeneous equation

$$(i\hbar \frac{\partial}{\partial t} - H(t))G(t, t') = \delta(t - t'). \quad (1.5)$$

The solution of the Schroedinger equation (1.1) can then be expressed as

$$|\Psi(t)\rangle = |\phi_i(t)\rangle + \int G(t, t_1)V_i(t_1)|\phi_i(t_1)\rangle dt_1 \quad (1.6)$$

where  $|\phi_i(t)\rangle$  is a given initial state. We may note here already that due to the implicit presence of the Heaviside theta-function in all the propagators (see, for example, the Volkov propagator given in the sequel) the time integration limits are always from a given initial time  $t_i$  to a given final time  $t_f$  since the limits of the intermediate time-integrations are automatically controlled by the propagators at the appropriate positions by themselves. Usually the interaction time interval  $t_f - t_i$  is taken to be long, e.g., from  $-\infty$  to  $+\infty$ . Note, however, that there is no difficulty in using the theory for interactions with any finite laser pulse, for during the rest of the time, from and to the long-time limits, the pulse could be assumed to be vanishingly small.

In general, as for the full wavefunction, we do not have explicit knowledge of the full propagator  $G(t, t')$ . Therefore, we intend to express it in terms of certain most relevant sub-propagators. Clearly, the two most relevant states in any quantum mechanical transition process are the initial state, in which the system is prepared, and the final state, in which the system is detected. Since in any ionisation process the final state interaction is governed by the long-range Coulomb interaction of the outgoing electron and the residual ion-core, it is highly desirable that the final state incorporates the long-range Coulomb interaction from the beginning.

Let us define a final reference Hamiltonian  $H_f(t)$  that incorporates the final-state Coulomb interaction in the presence of the laser field.  $H_f$ , and the corresponding final-state interaction  $V_f(t)$  are related to each other by the total Hamiltonian,  $H(t)$ ,

$$H(t) = H_f(t) + V_f(t) \quad (1.7)$$

Formally, the final state propagator is then defined as usual by

$$(i\hbar \frac{\partial}{\partial t} - H_f(t))G_f(t, t') = \delta(t - t') \quad (1.8)$$

Assuming for a moment that a suitable  $H_f(t)$  and  $G_f(t, t')$  for the present purpose could be found, the total  $G(t, t')$  can be re-expressed in terms of  $G_f(t, t')$  as

$$G(t, t') = G_f(t, t') + \int G_f(t, t_1)V_f(t_1)G(t_1, t')dt_1 \quad (1.9)$$

Substituting this in  $|\Psi(t)\rangle$  above we get a closed form expression of the full state vector in the form

$$\begin{aligned}
|\Psi(t)\rangle &= |\phi_i(t)\rangle + \int dt_1 G_f(t, t_1) V_i(t_1) |\phi_i(t_1)\rangle \\
&+ \int dt_2 dt_1 G_f(t, t_2) V_f(t_2) G(t_2, t_1) V_i(t_1) |\phi_i(t_1)\rangle \quad (1.10)
\end{aligned}$$

This formally closed form of the wavefunction of the interacting system has been originally derived and discussed in connection with non-sequential double ionization processes (see, review [14]). Here we shall make use of it for the problem at hand. In fact, the transition amplitude (or the S-Matrix element  $S_{fi}$ ) from an initial state,  $|\phi_i(t)\rangle$ , to a final state  $|\psi_f(t)\rangle$  of the system is given, by definition, by the projection of the final state on to the total wavefunction evolving from the initial state. Thus, using the above form of  $|\Psi(t)\rangle$ , we get

$$\begin{aligned}
S_{fi} &= \langle \psi_f(t) | \Psi(t) \rangle \\
&= \langle \psi_f(t) | \phi_i(t) \rangle + \int dt_1 \langle \psi_f(t_1) | V_i(t_1) | \phi_i(t_1) \rangle + \\
&+ \int dt_2 dt_1 \langle \psi_f(t_2) | V_f(t_2) G(t_2, t_1) V_i(t_1) | \phi_i(t_1) \rangle + \dots \quad (1.11)
\end{aligned}$$

This is a specially convenient general form of a transition amplitude from which to generate the desired expansion of the ionisation amplitude. Now,  $G(t, t')$  may be expanded in terms of *any* suitable intermediate sub-propagator and the corresponding intermediate interaction (without affecting the choice of the initial and the final states and the respective rest-interactions). This generates a series expansion of the strong-field S-matrix element of interest.

Before proceeding to derive the strong-field S-matrix series of present interest, we may pause here briefly to make a few observations on the general character of such series. Generally speaking, the strong-field S-matrix series are *not* perturbation series based on a “small parameter”. Thus, for example, the usual plane wave SFA expansion involves both the laser-atom interaction and the atomic potential. Indeed, most of its useful applications using the first and the second order terms have been for cases in which the laser field strength  $F$  had been *weaker* than the strength of the atomic potential or  $\frac{(eFa_0)}{(Ze^2/a_0)} < 1$ ,  $Z$  = nuclear charge; this is contrary to the view sometimes held that SFA is a perturbative expansion where the “small parameter” corresponds to the strength of the atomic potential (in comparison with the laser field strength).

More appropriately viewed, strong-field S-matrix series are *iterative* series, where each successive order of iteration corresponds to an additional intermediate interaction-event or “collision” (involving the active electron and, either the atomic potential or the laser-field, or both). With each increasing iteration order, the number of intermediate “collisions” to occur also increases and hence the probability of its significance for a given final event tends to decrease. Independent of this general but qualitative expectation, the final results can be tested for quantitative accuracy only *a posteriori* e.g. by comparison with accurate simulations (when feasible) and/or

with experimental data (when available). Another physically significant usefulness of such series is that they allow a *systematic* exploration of hypothesised mechanisms behind a strong-field phenomenon. This is possible due to the ability of the S-matrix series to systematically generate Feynman-like diagrams that can help to visualise the underlying mechanism(s) suggested by the diagrams, as well as to estimate their relative significance (see, e.g. [14]).

To continue with the problem at hand, we choose the strong-field Volkov propagator  $G_{Vol}(t, t')$  to expand the full  $G$  appearing in (1.11). The Volkov Hamiltonian is given by the interaction of the free-electron with the laser field only, or

$$H_{Vol}(t) = \left( \frac{\mathbf{p}_{op}^2}{2m} - \frac{e}{mc} \mathbf{A}(t) \cdot \mathbf{p} + \frac{e^2 A^2}{2mc^2} \right) \quad (1.12)$$

The solutions of the corresponding Schroedinger equation are easily found

$$\psi_{\mathbf{p}}(\mathbf{r}, t) = \langle \mathbf{r} | \mathbf{p} \rangle e^{-\frac{i}{\hbar} \int_{t'}^t \frac{p_{op}^2}{2m} dt''} \quad (1.13)$$

where  $\mathbf{p}_t \equiv (\mathbf{p} - \frac{e}{c} \mathbf{A}(t))$  and  $\langle \mathbf{r} | \mathbf{p} \rangle = e^{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}}$  is a plane wave of momentum  $\mathbf{p}$ .

The Volkov propagator  $G_{Vol}(t, t')$  is the solution of the inhomogeneous equation

$$(i\hbar \frac{\partial}{\partial t} - \left( \frac{\mathbf{p}_{op}^2}{2m} - \frac{e}{mc} \mathbf{A}(t) \cdot \mathbf{p} + \frac{e^2 A^2}{2mc^2} \right)) G_{Vol}(t, t') = \delta(t - t'). \quad (1.14)$$

which is therefore given explicitly by:

$$G_{Vol}(t, t') = -\frac{i}{\hbar} \theta(t - t') \sum_{\mathbf{p}} |\mathbf{p}\rangle e^{-\frac{i}{\hbar} \int_{t'}^t \frac{p_{op}^2}{2m} dt''} \langle \mathbf{p}| \quad (1.15)$$

Using the Volkov propagator we can expand

$$G(t, t') = G_{Vol}(t, t') + \int G_{Vol}(t, t_1) V_0(t_1) G_{Vol}(t_1, t') dt_1 + \dots \quad (1.16)$$

The intermediate interaction operator  $V_0(t)$  is accordingly defined by

$$\begin{aligned} V_0(t) &= H(t) - H_{Vol}(t) \\ &= \left( -\frac{Ze^2}{r} + V_{s.r.}(\mathbf{r}) \right) \end{aligned} \quad (1.17)$$

(which is time independent in the present case).

Since the initial state belongs to the atomic Hamiltonian  $H_a$ , therefore, the initial rest-interaction  $V_i(t)$  is, as indicated earlier, simply

$$\begin{aligned}
V_i(t) &= H(t) - H_a \\
&= \left( -\frac{e}{mc} \mathbf{A}(t) \cdot \mathbf{p}_{op} + \frac{e^2 A^2}{2mc^2} \right)
\end{aligned} \tag{1.18}$$

For the final state, we intend to take account of the long-range Coulomb interaction explicitly. One such state is the so-called ‘‘Coulomb-Volkov’’ state. It has been introduced a long time ago [15, 16] by taking the usual stationary Coulomb-wave and augmenting it heuristically by the time-dependent Volkov-phase:

$$\Phi_{\mathbf{p}}(\mathbf{r}, t) = \phi_{\mathbf{p}}^{(-)}(\mathbf{r}) \times e^{-\frac{i}{\hbar} \int_t^{\infty} \frac{p_{\mathbf{p}}'^2}{2m} dt'} \tag{1.19}$$

The stationary Coulomb waves,  $\phi_{\mathbf{p}}^{(-)}(\mathbf{r})$ , belong to the asymptotic atomic (or hydrogenic) Hamiltonian  $H_{Cou}$ :

$$\begin{aligned}
H_{Cou} &= H_a - V_{s.r.}(\mathbf{r}) \\
&= \left( \frac{\mathbf{p}_{op}^2}{2m} - \frac{Ze^2}{r} \right)
\end{aligned} \tag{1.20}$$

They are given by [17]

$$\phi_{\mathbf{p}}^{(-)}(\mathbf{r}) = \frac{1}{L^{\frac{3}{2}}} e^{\frac{\pi}{2} \eta_p} \Gamma(1 + i\eta_p) e^{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}} {}_1F_1(-i\eta_p, 1, -\frac{i}{\hbar}(pr + \mathbf{p} \cdot \mathbf{r})) \tag{1.21}$$

We have assumed them to be normalised in a large volume  $L^3$  with the understanding that, limit  $L \rightarrow \infty$ ,  $\sum_s(\dots) \equiv (\frac{L}{2\pi})^3 \int d^3s(\dots)$ ;  $\mathbf{p}_{op} \equiv -i\hbar\nabla$ , and  $\eta_p \equiv \frac{Z\hbar}{a_0 p}$  is the so-called Sommerfeld parameter;  $a_0 = \text{Bohr radius} = \frac{\hbar^2}{me^2}$ . Note that the ‘‘minus’’ Coulomb wave is chosen above, which is appropriate for the ionisation final state. We note in passing that for the laser assisted scattering problems the ‘‘plus’’ wave is also of interest; they are related to each other by the transformation  $\phi_{\mathbf{p}}^{(+)}(\mathbf{r}) = \phi_{-\mathbf{p}}^{(-)*}(\mathbf{r})$ .

To determine the associated final-state interaction we need to know the appropriate time-dependent Coulomb-Volkov Hamiltonian (call it  $H_{CV}(t)$ ). If it exists,  $H_{CV}(t)$  should be such, that the above defined Coulomb-Volkov state (1.19) should be a member of the complete set of linearly independent fundamental solutions of the associated Schroedinger equation.

### 1.3 Coulomb–Volkov Hamiltonian and Propagator

To determine the Hamiltonian  $H_{CV}(t)$  to which the Coulomb-Volkov state belongs, we introduce a vector operator defined by

$$\pi_c \equiv \sum_{\mathbf{s}} |\phi_{\mathbf{s}}\rangle \mathbf{s} \langle \phi_{\mathbf{s}}| \quad (1.22)$$

where  $|\phi_{\mathbf{s}}\rangle$  stands for the *Coulomb wave* (“+” or “-”) with momentum  $\mathbf{s}$ , cf. (1.21).

Consider next the exponential operator

$$T(\pi_c) = e^{i\alpha(t) \cdot \pi_c} \quad (1.23)$$

where  $\alpha(t) = \frac{e}{mc} \int^t \mathbf{A}(t') dt'$ . By expanding the exponential as a power series and using the projection operator nature of the individual terms, it can be reduced to the simple form

$$T(\pi_c) = 1 - \sum_{\mathbf{s}} |\phi_{\mathbf{s}}\rangle (1 - e^{i\alpha(t) \cdot \mathbf{s}}) \langle \phi_{\mathbf{s}}| \quad (1.24)$$

We can write the Coulomb-Volkov Hamiltonian  $H_{CV}(t)$  with the help of the operator  $\pi_c$ ,

$$H_{CV}(t) = \frac{\mathbf{p}_{op}^2}{2m} - \frac{Ze^2}{r} + \frac{e^2 A^2(t)}{2mc^2} - \frac{e}{mc} \mathbf{A}(t) \cdot \pi_c \quad (1.25)$$

The corresponding Schroedinger equation is

$$i\hbar \frac{\partial}{\partial t} \Phi_j(t) = \left( \frac{\mathbf{p}_{op}^2}{2m} - \frac{Ze^2}{r} + \frac{e^2 A^2(t)}{2mc^2} - \frac{e}{mc} \mathbf{A}(t) \cdot \pi_c \right) \Phi_j(t) \quad (1.26)$$

The complete set of linearly independent solutions of (1.26) is

$$|\Phi_j(t)\rangle = e^{-\frac{i}{\hbar} \int^t (E_j + \frac{e^2 A^2(t')}{2mc^2}) dt' + \frac{i}{\hbar} \alpha(t) \cdot \pi_c} |\phi_j\rangle \quad (1.27)$$

where  $j \equiv \mathbf{p}$ , stands for the momentum  $\mathbf{p}$  of the Coulomb wave state  $|\phi_{\mathbf{p}}^{(-)}\rangle$  and  $j \equiv D$  stands for the discrete indices of the bound states  $|\phi_D\rangle$  of the attractive Coulomb potential. To establish that (1.27) indeed satisfies (1.26), let us first consider the case  $\{j \equiv \mathbf{p}\}$  and use (1.24) to calculate,

$$\begin{aligned} e^{\frac{i}{\hbar} \alpha(t) \cdot \pi_c} |\phi_{\mathbf{p}}\rangle &= T(\pi_c) |\phi_{\mathbf{p}}\rangle \\ &= |\phi_{\mathbf{p}}\rangle - \sum_{\mathbf{s}} |\phi_{\mathbf{s}}\rangle (1 - e^{\frac{i}{\hbar} \alpha(t) \cdot \mathbf{s}}) \langle \phi_{\mathbf{s}} | \phi_{\mathbf{p}} \rangle \\ &= |\phi_{\mathbf{p}}\rangle - |\phi_{\mathbf{p}}\rangle (1 - e^{\frac{i}{\hbar} \alpha(t) \cdot \mathbf{p}}) \\ &= e^{\frac{i}{\hbar} \alpha(t) \cdot \mathbf{p}} |\phi_{\mathbf{p}}\rangle \end{aligned} \quad (1.28)$$

Also we have

$$-\frac{e}{mc}\mathbf{A}(t) \cdot \boldsymbol{\pi}_c|\phi_{\mathbf{p}}\rangle = -\frac{e}{mc}\mathbf{A}(t) \cdot \mathbf{p}|\phi_{\mathbf{p}}\rangle \quad (1.29)$$

Thus, substituting (1.27) in (1.26) for the continuum case, we get on the left hand side

$$l.h.s. = e^{-\frac{i}{\hbar}(\int^t(E_p + \frac{e^2 A^2(t')}{2mc^2})dt' - \alpha(t) \cdot \mathbf{p})}(E_p + \frac{e^2 A^2(t)}{2mc^2} - \dot{\alpha}(t) \cdot \mathbf{p})|\phi_{\mathbf{p}}\rangle \quad (1.30)$$

and on the right hand side,

$$r.h.s. = e^{-\frac{i}{\hbar}(\int^t(E_p + \frac{e^2 A^2(t')}{2mc^2})dt' - \alpha(t) \cdot \mathbf{p})}((\frac{\mathbf{p}_{op}^2}{2m} - \frac{Ze^2}{r}) + \frac{e^2 A^2(t')}{2mc^2} - \frac{e}{mc}\mathbf{A}(t) \cdot \mathbf{p})|\phi_{\mathbf{p}}\rangle \quad (1.31)$$

Noting that  $\dot{\alpha}(t) = \frac{e}{mc}\mathbf{A}(t)$  and  $H_{Cou}|\phi_{\mathbf{p}}\rangle = E_p|\phi_{\mathbf{p}}\rangle$ , where,  $E_p = \frac{p^2}{2m}$ , one easily finds from above that the  $l.h.s = r.h.s$  and hence the given solution is exactly fulfilled.

In a similar way it is easily seen that

$$\begin{aligned} T(\pi_c)|\phi_D\rangle &= |\phi_D\rangle - \sum_s |\phi_s\rangle(1 - e^{\frac{i}{\hbar}\alpha(t) \cdot \mathbf{s}})\langle\phi_s|\phi_D\rangle \\ &= |\phi_D\rangle + 0 \end{aligned} \quad (1.32)$$

since, the overlap integral between the discrete and the continuum eigenstates of the Coulomb Hamiltonian vanish by orthogonality,  $\langle\phi_s|\phi_D\rangle = 0$ . Hence, on substituting (1.27) in (1.26) in the discrete case we get

$$l.h.s. = e^{-\frac{i}{\hbar}(\int^t(E_D + \frac{e^2 A^2(t')}{2mc^2})dt' + 0)}(E_D + \frac{e^2 A^2(t)}{2mc^2} + 0)|\phi_D\rangle \quad (1.33)$$

and

$$r.h.s. = e^{-\frac{i}{\hbar}(\int^t(E_D + \frac{e^2 A^2(t')}{2mc^2})dt' + 0)}((\frac{\mathbf{p}_{op}^2}{2m} - \frac{Ze^2}{r}) + \frac{e^2 A^2(t')}{2mc^2} + 0)|\phi_D\rangle \quad (1.34)$$

Moreover,  $(\frac{\mathbf{p}_{op}^2}{2m} - \frac{Ze^2}{r})|\phi_D\rangle = E_D|\phi_D\rangle$  and, therefore, the  $l.h.s = r.h.s$  and the verification is complete.

To summarise, the complete set of solutions of the CV-Schrodinger equation defined by (1.26) is given explicitly for the continuum case by

$$\Phi_{\mathbf{p}}^{(-)}(\mathbf{r}, t) = \phi_{\mathbf{p}}^{(-)}(\mathbf{r})e^{-\frac{i}{\hbar}(\int^t(\frac{p^2}{2m} + \frac{1}{2c^2}A(t')^2 - \frac{e}{c}\mathbf{A}(t') \cdot \mathbf{p})dt'} \quad (1.35)$$

and for the discrete case by



$$\Phi_D(\mathbf{r}, t) = \phi_D(\mathbf{r}) e^{-\frac{i}{\hbar} \int^t (\frac{p^2}{2m} + \frac{1}{2c^2} A(t')^2) dt'} \quad (1.36)$$

where we may recall that [17]

$$\langle \mathbf{r} | \phi_{\mathbf{p}}^{(-)} \rangle = \frac{1}{L^{3/2}} e^{\frac{\pi \eta_p}{2}} \Gamma(1 + i\eta_p) e^{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}} {}_1F_1(-i\eta_p, 1, -\frac{i}{\hbar} (pr + \mathbf{p} \cdot \mathbf{r})) \quad (1.37)$$

with  $\eta_p = \frac{Z\hbar}{pa_0}$ , and the well known hydrogenic bound states,

$$\begin{aligned} \phi_{D \equiv (n, l, m)}(\mathbf{r}) &= N_{nl} R_{nl}(r) Y_{lm}(\theta, \phi) \\ R_{nl}(r) &= (2\kappa_n r)^l e^{-\kappa_n r} F_1(-n + l + 1, 2l + 2, 2\kappa_n r) \\ N_{nl} &= \frac{(2\kappa_n)^{3/2}}{\Gamma(2l + 2)} \sqrt{\frac{\Gamma(n + l + 1)}{2n\Gamma(n - l)}} \end{aligned} \quad (1.38)$$

with  $\kappa_n \equiv \frac{Z}{na_0} = \sqrt{\frac{-2mE_D}{\hbar^2}}$ .

Having thus found the explicit form of both  $H_{CV}(t)$ , (1.25), and the complete set of solutions [(1.27) or, (1.35) and (1.36)] of the Coulomb-Volkov Schrodinger equation, (1.26), we may now write down the associated Coulomb-Volkov propagator  $G_{CV}(t, t')$  explicitly,

$$\begin{aligned} G_{CV}(t, t') &= -\frac{i}{\hbar} \theta(t - t') \\ &\times \{ \sum_{\mathbf{p}} |\phi_{\mathbf{p}}\rangle e^{-\frac{i}{\hbar} \int_{t'}^t (\frac{\mathbf{p}^2}{2m} + \frac{e}{2m} A(t'')^2) dt''} \langle \phi_{\mathbf{p}}| \\ &+ \sum_{nlm} |\phi_{nlm}\rangle e^{-\frac{i}{\hbar} \int_{t'}^t (E_{nl} + \frac{e^2 A^2(t'')}{2mc^2}) dt''} \langle \phi_{nlm}| \} \end{aligned} \quad (1.39)$$

## 1.4 Coulomb-Volkov S-Matrix Series

We are now in a position to obtain the desired S-matrix amplitude. From the knowledge of  $H_{CV}(t)$  obtained above the rest-interaction in the final-state turns out to be,

$$\begin{aligned} V_{CV}(t) &= H(t) - H_{CV}(t) \\ &= (-\frac{e}{mc} \mathbf{A}(t) \cdot (\mathbf{p}_{\text{op}} - \pi_{\mathbf{c}}) + V_{s,r}(\mathbf{r})) \end{aligned} \quad (1.40)$$

Therefore, substitutions of the initial and the final rest-interactions as well as the expansion of  $G(t, t')$  in terms of the Volkov propagator and the intermediate rest-interaction  $V_0(\mathbf{r}) = (-\frac{Ze^2}{r} + V_{s,r}(\mathbf{r}))$  into the amplitude expression (1.11), immediately yield:

$$\begin{aligned}
S_{fi} = & \langle \Phi_{\mathbf{p}}(t) | \phi_i(t) \rangle \\
& - \frac{i}{\hbar} \int dt_1 \langle \Phi_{\mathbf{p}}(t_1) | V_i(t_1) | \phi_i(t_1) \rangle \\
& - \frac{i}{\hbar} \int dt_2 dt_1 \langle \Phi_{\mathbf{p}}(t_2) | (-\frac{e}{mc} \mathbf{A}(t_2) \cdot (\mathbf{p}_{op} - \pi_c) + V_{s.r.}(\mathbf{r}_2)) \times \\
& \times G_{Vol}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) V_i(t_1) | \phi_i(t_1) \rangle \\
& \dots
\end{aligned} \tag{1.41}$$

Thus, finally, we have arrived at the desired systematic S-matrix series for the strong-field ionisation amplitude, which systematically accounts for the final state long range Coulomb interaction through the Coulomb-Volkov state in all orders. We quote the first three terms more explicitly and, give the rule of construction for all the higher order terms of the series:

$$S_{fi} = \sum_{n=0}^{\infty} S_{fi}^{(n)} \tag{1.42}$$

where,

$$S_{fi}^{(0)} = \langle \Phi_{\mathbf{p}}(\mathbf{r}, t) | \phi_i(\mathbf{r}, t) \rangle \tag{1.43}$$

$$S_{fi}^{(1)} = -\frac{i}{\hbar} \int dt_1 \langle \Phi_{\mathbf{p}}(\mathbf{r}_1, t_1) | (-\frac{e}{mc} \mathbf{A}(t_1) \cdot \mathbf{p}_{op} + \frac{e^2 A^2(t_1)}{2mc^2}) | \phi_i(\mathbf{r}_1, t_1) \rangle \tag{1.44}$$

$$\begin{aligned}
S_{fi}^{(2)} = & -\frac{i}{\hbar} \int dt_2 dt_1 \langle \Phi_{\mathbf{p}}(\mathbf{r}_2, t_2) | (-\frac{e}{mc} \mathbf{A}(t_2) \cdot (\mathbf{p}_{op} - \pi_c) + V_{s.r.}(\mathbf{r}_2)) G_{Vol}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) \\
& \times (-\frac{e}{c} \mathbf{A}(t_1) \cdot \mathbf{p}_{op} + \frac{e^2 A^2(t_1)}{2mc^2}) | \phi_i(\mathbf{r}_1, t_1) \rangle
\end{aligned} \tag{1.45}$$

$$\begin{aligned}
S_{fi}^{(3)} = & -\frac{i}{\hbar} \int dt_3 dt_2 dt_1 \langle \Phi_{\mathbf{p}}(\mathbf{r}_3, t_3) | (-\frac{e}{mc} \mathbf{A}(t_3) \cdot (\mathbf{p}_{op} - \pi_c) + V_{s.r.}(\mathbf{r}_3)) \\
& \times G_{Vol}(\mathbf{r}_3, t_3; \mathbf{r}_2, t_2) (-\frac{Ze^2}{r_2} + V_{s.r.}(\mathbf{r}_2)) G_{Vol}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) \\
& \times (-\frac{e}{mc} \mathbf{A}(t_1) \cdot \mathbf{p}_{op} + \frac{e^2 A^2(t_1)}{2mc^2}) | \phi_i(\mathbf{r}_1, t_1) \rangle \\
& \dots
\end{aligned} \tag{1.46}$$

where the angle brackets stand for the integration with respect to the space coordinates and “...” stands for the higher orders terms. The higher order terms can be written down easily, if required, for they follow the same pattern as the third order term but are simply extended by an extra intermediate factor  $G_{Vol} V_0$  and an extra time integration for each successive order, to all orders.

## 1.5 Strong-Field S-Matrix for Short-Range Potentials

Before ending this report it is interesting to consider the S-matrix expansion of the strong-field amplitude in the presence of an asymptotically short range potential. This can be obtained simply by taking the limit  $Z = 0$  in the result derived above. In this limit the Coulomb waves  $\phi_{\mathbf{p}}(\mathbf{r})$  reduce to the plane waves  $e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}$  and the Coulomb-Volkov state  $\Phi_{\mathbf{p}}(\mathbf{r}, t)$  (1.19) reduces to the Volkov state (1.13). This implies that the factor with the final state interaction in all terms, beginning with the second order term, reduces to the short range potential  $V_{s.r.}(\mathbf{r})$  only, due to the following simplification

$$\begin{aligned} \langle \mathbf{p} | (-\frac{e}{mc} \mathbf{A}(t) \cdot (\mathbf{p}_{op} - \pi_c) + V_{s.r.}(\mathbf{r})) &= (-\frac{e}{mc} \mathbf{A}(t) \cdot (\mathbf{p} - \mathbf{p}) \langle \mathbf{p} | + \langle \mathbf{p} | V_{s.r.}(\mathbf{r})) \\ &= \langle \mathbf{p} | V_{s.r.}(\mathbf{r}) \end{aligned} \quad (1.47)$$

Also, the intermediate interaction  $V_0$  in all terms (from the second order term onwards) for  $Z = 0$  reduces to the short-range potential  $V_{s.r.}(\mathbf{r})$  only. Hence, in general, for  $Z \equiv 0$ , the Coulomb-Volkov S-matrix series, (1.41), goes over to the simpler series

$$\begin{aligned} S_{fi}(Z = 0) &= \langle \psi_{\mathbf{p}}(t) | \phi_i(t) \rangle \\ &- \frac{i}{\hbar} \int dt_1 \langle \psi_{\mathbf{p}}(t_1) | V_i(t) | \phi_i(t) \rangle \\ &- \frac{i}{\hbar} \int dt_2 dt_1 \langle \psi_{\mathbf{p}}(t_2) | V_{s.r.}(\mathbf{r}_2) G_{Vol}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) V_i(t_1) | \phi_i(t) \rangle \\ &- \frac{i}{\hbar} \int dt_3 dt_2 dt_1 \langle \psi_{\mathbf{p}}(t_3) | V_{s.r.}(\mathbf{r}_3) G_{Vol}(\mathbf{r}_3, t_3; \mathbf{r}_2, t_2) V_{s.r.}(\mathbf{r}_2) \\ &\quad \times G_{Vol}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) V_i(t_1) | \phi_i(t_1) \rangle \\ &+ \dots \end{aligned} \quad (1.48)$$

Equation (1.48) provides a strong-field S-matrix expansion when there is no long-range Coulomb interaction preset asymptotically. This occurs with all asymptotically neutral systems with effective core charge  $Z = 0$  (as seen by the ejected electron) e.g. for the case of electron-detachment from negative ions. Equation (1.48) is apparently analogous in structure to the usual SFA with the plane-wave Volkov final state. Note, however, that in (1.48) the plane-wave Volkov final state and the short-range potential  $V_{s.r.}$ , appear self-consistently together.

## 1.6 Concluding Remarks

We may end this report with a few short remarks.

(a) For the sake of concreteness we have presented the result starting with the Schroedinger equation of the interacting system in the minimal coupling gauge (so-called velocity gauge). A similar result can be derived in the same way (or by a gauge transformation) starting from the Schroedinger equation in the so-called length gauge. This and the issue of gauge invariance of the theory will be presented and discussed elsewhere.

(b) It is expected that the present theory would be helpful in clarifying a number of issues of much current interest in strong-field physics involving (i) the shape of the so-called “low energy structure” (LES) [18], (ii) the number of peaks associated with the “very low energy structures” (VLES) [19, 20], (iii) origin of the “zero energy structure” (ZES) [21], and (iv) possible existence of an as yet unknown “threshold law” for the energy dependence of the strong-field ionization probability. Most or all of these issues possibly depend crucially on the role of the long-range final state Coulomb interaction specially in the low energy regime (e.g. c.f. [22]).

(c) The explicit expression of the Coulomb-Volkov propagator (or Green’s function)  $G_{CV}(t, t')$  given here suggests that the theory also would be useful for strong-field processes involving excitation of the discrete states, either as a final state, or as intermediate mediating states, or both, for example, in connection with the so-called “frustrated ionization” (e.g. [23]) in strong fields.

(d) We may point out that the terms of the S-matrix series (1.42), for example, the amplitudes  $S_{if}^{(1)}$  and  $S_{if}^{(2)}$ , could be evaluated by a combination of stationary phase method and numerical evaluation, provided the coordinates dependent Coulomb integrals can be evaluated analytically, for example by Norsieck’s method [24]. The Coulomb integral of the first order amplitude (and of the first factor of the second order amplitude) are of the form

$$M_{\mathbf{p},i}^{(1)} = \int \phi_{\mathbf{p}}^{(-)*}(\mathbf{r}) \left(-\frac{e}{mc} \mathbf{A}(t) \cdot \mathbf{p}_{op}\right) e^{-\kappa r} d^3 r \quad (1.49)$$

where  $\eta(p) \equiv \frac{Z\hbar}{pa_0}$ . The second Coulomb integral of the 2nd order amplitude is of the form

$$\begin{aligned} M_{\mathbf{p},\mathbf{k}}^{(2)} &= \int \phi_{\mathbf{p}}^{(-)*}(\mathbf{r}) \left(-\frac{e}{mc} \mathbf{A}(t) \cdot (\mathbf{p}_{op} - \pi_c)\right) e^{i\mathbf{k}\cdot\mathbf{r}} d^3 r \\ &= \left(-\frac{e}{mc} \mathbf{A}(t) \cdot (\mathbf{k} - \mathbf{p})\right) \int \phi_{\mathbf{p}}^{(-)*}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3 r \end{aligned} \quad (1.50)$$

They have the same form as of the following two prototypical integrals which we give explicitly below:

$$\begin{aligned} I_1 &= \int e^{-is\cdot\mathbf{r}} {}_1F_1(i\eta_s, 1, i(sr + \mathbf{s} \cdot \mathbf{r})) (\boldsymbol{\varepsilon} \cdot \mathbf{p}_{op}) e^{-\kappa r} d^3 r \\ &= 8\pi\hbar\kappa(1 + i\eta_s)(\boldsymbol{\varepsilon} \cdot \mathbf{s}) / ((\kappa + is)^{(2-i\eta_s)} (\kappa - is)^{(2+i\eta_s)}) \end{aligned} \quad (1.51)$$

$$\begin{aligned}
I_2 &= (\boldsymbol{\varepsilon} \cdot (\mathbf{k} - \mathbf{s})) \times \lim_{\lambda \rightarrow 0} \int e^{-is \cdot \mathbf{r}} {}_1F_1(i\eta_s, 1, i(sr + \mathbf{s} \cdot \mathbf{r})) e^{i\mathbf{k} \cdot \mathbf{r}} e^{-\lambda r} d^3r \\
&= (\boldsymbol{\varepsilon} \cdot \mathbf{q}) \times \frac{8\pi s \eta_s}{q^2(q^2 + 2\mathbf{q} \cdot \mathbf{s})} \left( \frac{q^2}{q^2 + 2\mathbf{q} \cdot \mathbf{s}} \right)^{i\eta_s}
\end{aligned} \tag{1.52}$$

where,  $\mathbf{q} \equiv \mathbf{k} - \mathbf{s}$ ,  $\eta_s = \frac{Z}{sa_0}$ , and  $\boldsymbol{\varepsilon}$  stands for an unit vector. The additional integration over the intermediate momentum  $\mathbf{k}$  can be performed e.g. by the stationary phase method (or otherwise), and the first time-integration can be done either analytically or by the stationary phase method, while the second time-integration can be done e.g. numerically. (Application of the theory to the observed low energy structures/phenomena [18–21] with more details of the calculations and discussions of the results will be presented elsewhere).

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