Limits of a stationary phase method for ionization of atoms in strong laser fields

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Abstract

A stationary phase approach to a typical $S$-matrix expansion for atomic ionization in strong laser fields is examined with respect to its range of validity.

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1. Introduction

Ionization of an atom induced by an intense laser field and related processes, such as high harmonic generation and nonsequential double ionization, have been studied extensively during the past two decades. In the domain of nonperturbative electron–field interaction exact calculations of the process probability by direct numerical solution of the associated Schrödinger equation of the system of interest require large computational effort. Hence, systematic approximation methods, such as the $S$-matrix theory, are often used for an estimation of the transition amplitude. For example, one of the most well-known formula for the total rate of ionization of atoms, the so-called Keldysh–Faisal–Reiss (KFR) formula [1], can be obtained as the leading term of a $S$-matrix expansion.

In the application of $S$-matrix theory to strong-field processes often Fourier-type integrals with large parameters in the exponent occur. Such integrals can asymptotically be reduced to the contribution of a few terms by means of the stationary phase method (e.g., [2,3]). The method has been used in the case of high harmonic generation [4], high-energy above threshold ionization [5–7] and nonsequential double ionization [8,9] to approximately evaluate terms of the respective $S$-matrix expansion.

Below we examine the range of validity of the stationary phase ansatz for a typical strong-field $S$-matrix expansion. To this end, we apply the stationary phase method to the calculation of the total rate of ionization of hydrogen atom within the first-order
KFR theory. Then we compare the results obtained using this approximation with those of the exact evaluation of the KFR ionization rate.

2. Application of the stationary phase method

Using the standard KFR ansatz of first order for the wavefunction of an initially bound electron subjected to intense laser radiation, the transition amplitude to a wavefunction of an initially bound electron subjected to intense laser radiation, the transition amplitude to a

Volkov state at time \( t \) can be written as (Hartree atomic units, \( e = \hbar = m = 1 \) are used, e.g., [10])

\[
A^{(1)}_{fi}(t) = -i \int_{t_i}^{t} dt_1 \left[ \phi_k^V(t_1) - \frac{\mathbf{p} \cdot \mathbf{A}(t_1)}{c} \right]
+ \frac{A^2(t_1)}{2e^2} |\phi_0(t_1)|^2,
\]

where \( \mathbf{A}(t) \) denotes the vector potential of the electron–field interaction in the dipole approximation, \( \phi_0 \) is the initial state wavefunction and \( \phi_k^V \) is the Volkov wavefunction of momentum \( k \). We take the absolute square of the amplitude and sum over all final state momenta to obtain

\[
P_{ion}^{(1)}(t) = \int_{t_0}^{t} dt_1 \int_{t}^{t_2} d\mathbf{k} V(\mathbf{k}, t_1) V(\mathbf{k}, t_2)
\times \exp(-iS(\mathbf{k}, t_1, t_2)) |\phi_0(\mathbf{k})|^2,
\]

(2)

where \( V(\mathbf{k}, t) = -\mathbf{k} \cdot \mathbf{A}(t)/c + A^2(t)/2e^2 \) and \( \phi_0(\mathbf{k}) \) is the Fourier transform of the initial state wavefunction. The phase \( S(\mathbf{k}, t_1, t_2) \) consists of the joint action of the Volkov electron in the velocity gauge and the ionization potential \( I_p \):

\[
S(\mathbf{k}, t_1, t_2) = \int_{t_1}^{t_2} dt' \left[ \frac{1}{2} \left( \mathbf{k}(t') - \frac{\mathbf{A}(t')}{c} \right)^2 + I_p \right].
\]

(3)

For a linearly polarized laser field with polarization direction along the \( z \)-axis, we separate in Eq. (2) the \( \mathbf{k} \)-integration into a part along the \( z \)-axis and those perpendicular to it. At high laser intensities the vector potential is assumed to be large and the stationary phase method (e.g., [2,3]) is applied to evaluate the \( k_z \)-integral. There is one stationary point \( k_z \) for each pair \((t_1, t_2)\),

\[
k_z(t_1, t_2) = \frac{1}{ct} \int_{t_1}^{t_2} dt' A(t'),
\]

(4)

and we get

\[
P_{ion}^{(1)}(t) \approx 2\pi^2 \int_{t_0}^{t} dt_1 \int_{t}^{t_2} d\mathbf{k} \frac{V(k_z, t_1) V(k_z, t_2)}{\sqrt{2\pi i \tau}}
\times \exp(-iS(k_z, t_1, t_2)) I(k_z),
\]

(5)

where

\[
I(k_z) = \int d(\mathbf{k}_\perp) |\phi_0(k_\perp, k_z)|^2 \exp\left(-i\frac{\tau g_4(k_z, \tau)}{2}\right).
\]

(6)

\[
\tau = t_2 - t_1 \quad \text{and}
\]

\[
S(k_z, t_1, t_2) = \left( I_p - \frac{k_z^2}{2}\right)\tau + \frac{1}{2c^2} \int_{t_1}^{t_2} dt' A^2(t').
\]

(7)

Using

\[
\phi_0(r) = Z \sqrt{\frac{\pi}{\lambda}} \exp(-\lambda r) Y_{00}(\hat{r}), \quad \lambda = Z
\]

for the ground state of hydrogenic atoms, we evaluate

\[
I(k_z) = 64\pi \lambda^5 g_4(k_z, \tau)
\]

with

\[
g_4(k_z, \tau) = \int_0^\infty dx \left( \frac{1}{x + \beta^4} \right)^4 e^{-i\mu x}
\]

\[
= \frac{U(1, -2, i\mu\beta)}{\beta^5} = \exp(i\mu\beta) \frac{E_4(i\mu\beta)}{\beta^5},
\]

(8)

where \( \beta = \lambda^2 + k_z^2 > 0 \) and \( \mu = \frac{\tau}{2} \). \( U(1, -2, z) \) denotes the confluent hypergeometric function, which can be expressed for purely imaginary arguments by means of the fourth exponential integral function \( E_4 \).

Using the result in Eq. (5), we get

\[
P_{ion}^{(1)}(t) \approx 16\lambda^5 \int_{t_0}^{t} dt_1 \int_{t}^{t_2} \frac{V(k_z, t_1) V(k_z, t_2) g_4(k_z, \tau)}{\sqrt{2\pi i \tau}}
\times \exp(-iS(k_z, t_1, t_2))
\]

\[
\int \frac{d(\mathbf{k}_\perp)}{\sqrt{2\pi i \tau}}
\]

\[
\times \exp(-iS(k_z, t_1, t_2)) I(k_z).
\]

(9)
\[ \Gamma_\text{eff}^+ = \frac{1}{T_p} \ln(1 - P_{\text{ion}}(T_p)) \]  

(10)

using \( P_{\text{ion}} \approx P_{\text{ion}}^{(1)} \) (for \( P_{\text{ion}}^{(1)} \leq 1 \)).

In the last step we have ordered the time integrations so that \( \tau > 0 \). The integrand contains an integrable 1/2 singularity and can be evaluated by direct numerical integration, since for small imaginary phase method to the final expression, if in Eq. (2) the stationary phase integration exactly and applying the stationary phase method is applied to the \( k \)-integration in all three dimensions. Usually the integrations over \( t_1 \) and \( t_2 \) are then performed by introducing a cutoff parameter [4]. As shown here, this additional approximation can be avoided in the case of linear polarization by performing the \( k_\perp \)-integration exactly and applying the stationary phase method to the \( k_\parallel \)-integration only. We may further stress that, in fact, for linear polarization an asymptotically large parameter in the phase is present in the field direction only.

3. Results and discussion

Since we have taken into account the first order term of the \( S \)-matrix series only, \( P_{\text{ion}}^{(1)} \) is not the total ionization probability, e.g., it is not restricted by unity. But, it is possible to determine a well-defined ionization rate, since \( P_{\text{ion}}^{(1)} \) is found to depend linearly on the interaction time. This is exemplified in Fig. 1, where \( P_{\text{ion}}^{(1)}(T_p) \) is shown as a function of the pulse length \( T_p \), for an intense laser pulse at 800 nm and \( 1.053 \times 10^{15} \) W/cm\(^2\) having a \( \sin^2 \)-pulse shape.

Thus, the validity of the present stationary phase ansatz can be examined by evaluation of effective rates per pulse of length \( T_p \), defined by [11]

\[ \Gamma_\text{eff}^+ = \frac{1}{T_p} \ln(1 - P_{\text{ion}}(T_p)) \]  

(10)

which is solved under the constraint \( P_{\text{ion}}(t = 0) = 0 \). The result is used in Eq. (10) to obtain the effective ionization rate for a finite pulse of length \( T_p \). In Fig. 2 we compare the effective rates as a function of the peak intensity obtained by using the stationary phase method (open diamonds) with the exact KFR results (lines) at different wavelengths between 400 and 1400 nm. The temporal profile of the pulse has been chosen to have a \( \sin^2 \)-shape of 10-cycle duration. It is seen from the figure that the results obtained using the stationary phase method agree well with the exact KFR rates, as expected, at high intensities. Below a critical intensity the approximative results are
found to systematically overestimate the exact effective rates. The results indicate that the application of the stationary phase method in a typical $S$-matrix expansion is justified as long as the intensity of the laser pulse is above mid of $10^{13}$ W/cm$^2$.

4. Summary

In conclusion, we have examined a stationary phase approximation to the first-order KFR theory of atomic ionization in a strong linearly polarized laser field. The stationary phase method has been applied to the momentum direction along the polarization direction of the field only, in order to avoid a typical non-integrable singularity in the final expression for the total ionization rate. It is found that the approximation is valid for intensities above mid of $10^{13}$ W/cm$^2$.

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