Reply to "Comment on 'Generalization of Keldysh's theory'"

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In response to the preceding Comment, we present the intermediate steps skipped in our mathematical derivation of the Keldysh integral using the residue integration method in the complex domain. We describe in detail the pole structures and the closed contour for performing the residue calculation. We analyze and discuss the implications of the analytic formula together with representative numerical calculations. The present analysis completes and validates our mathematical analysis of the Keldysh integral.

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With the availability of intense lasers of high repetition rate, there have been considerable activities in the study of the nonlinear response of atoms and molecules subjected to strong electromagnetic radiation [1]. Nonperturbative theoretical studies based on the strong field approximation have been traditionally employed to understand the fundamental multiphoton processes involved in the matter-radiation interactions. Among them Keldysh theory $\begin{bmatrix} 2 \end{bmatrix}$ plays an important role and is still being used to interpret many experimental observations. Keldysh has derived an analytical expression for the photoionization rate of a hydrogen atom in the linearly polarized strong laser field using the length gauge [2]. Faisal and also Reiss have introduced the S-matrix formalism using the velocity gauge [3]. In particular Reiss has developed an efficient method to calculate the ionization rate using generalized Bessel functions [3]. A generalized strong field approximation using semiclassical complex saddle point methods has also been employed to study the tunneling-rescattering processes such as high harmonic generation (HHG) [4] and above-threshold ionization (ATI) [5]. Recently, generalizations of Keldysh theory beyond the original range of applicability have been proposed $\begin{bmatrix} 6-8 \end{bmatrix}$.

In this Reply to the preceding Comment [9] we complete our derivation of Keldysh's integral using the residue integration method by explicitly showing the closed contour and the pole structure. Keldysh's original theory [2] adopted the length gauge, and the ionized electron is described by the Volkov wave function. The photoionization rate W_0 of the electron in the ground state of a hydrogen atom in the presence of a linearly polarized strong laser field $\vec{F} \cos \omega t$ is given by

$$W_0 = \frac{2\pi}{\hbar} \sum_{n > [(I_0 + U_p)/(\hbar\omega)]} \int \frac{d^3 p}{(2\pi\hbar)^3} |L(\vec{p})|^2 \\ \times \delta \left(\frac{p^2}{2m_e} + I_0 + U - n\hbar\omega\right), \tag{1}$$

where $I_0 = \hbar^2 / (2m_e a_0^2)$ is the ionization potential and

 $U = (eF)^2 / (4m_e \omega^2)$ is the pondermotive energy. The Keldysh integral $L(\vec{p})$ is given by the integral over $\theta = \omega t$,

$$L(\vec{p}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \cos \theta V_0 \left(\vec{p} + \frac{e}{\omega} \vec{F} \sin \theta \right)$$
$$\times \exp\left(\frac{i}{\hbar\omega} [n\hbar\omega\theta - \xi\cos\theta - U\sin\theta\cos\theta]\right), \quad (2)$$

with $V_0(\vec{p}) = K_{1s}epF \cos \theta_{pF}[I_0 + p^2/(2m_e)]^{-3}$, $K_{1s} = -32i\sqrt{\pi a^7}I_0^{-3}\hbar^{-1}$, and $\xi = epF \cos \theta_{pF}/(m_e\omega)$, where θ_{pF} is the angle between \vec{p} and \vec{F} , and $n\hbar\omega = I_0 + U + p^2/2m_e$. We compute Eq. (2) by first transforming it into a contour integral form in $u = \sin \theta$ domain. This transformation has to be done with care concerning the multivalued functional relation. Following Keldysh [2], the integral with respect to u is taken along a closed contour enclosing the segment [-1,1], which forms a branch cut to make the integrand single valued. For multiphoton ionizations, the integrand is highly oscillating and this is the theoretical background for using the saddle point method to approximate the integral. However, because the poles and the saddle points coincide in the Keldysh integral, we argue that the residue integration method should be more appropriate in dealing with the singularities. To compute Eq. (2), we consider the contour integral

$$L_{C}(\vec{p}) = \frac{1}{2\pi} \int_{C} du V_{0} \left(\vec{p} + \frac{e}{\omega} \vec{F} u \right) \exp\left(\frac{i}{\hbar \omega} j(u) \right), \quad (3)$$

where

$$j(u) = n\hbar\omega \frac{1}{i}\ln[iu + (-i\sqrt{u-1}\sqrt{u+1})] - \xi(-i\sqrt{u-1}\sqrt{u+1}) - Uu(-i\sqrt{u-1}\sqrt{u+1})$$
(4)

and *C* stands for a contour consisting of the contours C_{ε} , C_{\pm} , L_{\pm} , and C_R shown in Fig. 1. In addition, j(u) stands for an analytically continued expression of the function j(u) on C_{\pm} and is defined in the whole *u* plane so that the residue theorem can be properly applied. By considering that the contributions from C_{ε} and L_{\pm} are zero, we find that the Keldysh

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FIG. 1. Contour integral for $L(\vec{p})$ in the *u* domain is depicted. The poles of $V_0(\vec{p} + \frac{e}{\omega}\vec{F}u)$ lie at $u=u_{\pm}$ and there is a branch cut between $-1 \le u \le 1$ on the real axis.

integral $L(\vec{p})$ in Eq. (2) can be given, in terms of $L_C(\vec{p})$ and $L_R(\vec{p})$, by

$$L(\vec{p}) = L_C(\vec{p}) - L_R(\vec{p}) = \sum_{k=+,-} L_C(\vec{p},k) - L_R(\vec{p}), \quad (5)$$

where

$$L_C(\vec{p},k) = 2\pi i \operatorname{Res}_{u=u_k} \frac{1}{2\pi} V_0 \left(\vec{p} + \frac{e}{\omega} \vec{F} u \right) \exp\left(\frac{i}{\hbar \omega} j(u)\right) \quad (6)$$

and

$$L_{R}(\vec{p}) = \frac{1}{2\pi} \int_{C_{R}} du V_{0} \left(\vec{p} + \frac{e}{\omega} \vec{F} u \right) \exp\left(\frac{i}{\hbar \omega} j(u) \right).$$
(7)

The poles at $u=u_{\pm}$ in $L_C(\vec{p},k)$ are rank-3 poles and given by $u_{\pm} = \frac{\omega}{eF} [-p \cos \theta_{pF} \pm i \sqrt{2m_e I_0 + p^2 \sin^2 \theta_{pF}}]$. We note that the residue on the upper half plane gives the same result reported by Mishima *et al.* [6]. However, the residue on the lower half plane was not taken into account in the original Keldysh theory [2] and that by Mishima *et al.* [6]. Gribakin and Kuchiev included these two poles and dropped off the other two poles which will not appear in θ domain but appear in θ domain [7,8].

The term $L_C(\vec{p},k)$ in Eq. (6) is calculated as

$$L_{C}(\vec{p},k) = \lim_{u \to u_{k}} \frac{1}{2!} \frac{d^{2}}{du^{2}} \left[(u - u_{k})^{3} \frac{1}{2\pi} V_{0} \left(\vec{p} + \frac{e}{\omega} \vec{F}u \right) \exp\left(\frac{i}{\hbar\omega} j(u) \right) \right]$$
$$= \sum_{k=+,-} \frac{-m_{e} K_{1s}}{4U(u_{+} - u_{-})\hbar\sqrt{1 - u_{k}^{2}}} \exp\left(\frac{i}{\hbar\omega} j(u_{k})\right). \tag{8}$$

For the calculation of $L_R(\vec{p})$ in Eq. (7), we need to expand $V_0(\vec{p} + \frac{e}{\omega}\vec{F}u)\exp(\frac{i}{\hbar\omega}j(u))$ in powers of u and u^{-1} , and perform the θ integral by putting $u=R\exp(i\theta)$. We obtain

$$L_{R}(\vec{p}) = \frac{1}{2\pi} \int_{C_{R}} du V_{0} \left(\vec{p} + \frac{e}{\omega} \vec{F}u \right) \exp\left(\frac{i}{\hbar\omega} j(u) \right)$$

$$= i \frac{m_{e} \hbar \omega^{2} K_{1s}}{8U^{3}} \sum_{l, j_{1}, j_{2}, m=0}^{\infty} a_{l}(n) b_{j_{1}}(b) c_{j_{2}}(c) C(m)$$

$$\times \{ bB_{m'}(b, c) + 4cB_{m'-1}(b, c) \}, \qquad (9)$$

where $m'=m+5+n+2l+j_1+2j_2$, $b=\xi/(\hbar\omega)$, and $c = U/(\hbar\omega)$. Here C(m), $a_l(n)$, $B_{m'}(b,c)$, $b_{j_1}(b)$, and $c_{j_2}(c)$ are given as

$$C(m) = \frac{1}{2(x-y)^5} [(m+1)(m+2)(x^{m+5} - y^{m+5}) + 2(m+1)(m+5)xy(x^{m+3} - y^{m+3}) + (m+4)(m+5)x^2y^2(x^{m+1} - y^{m+1})]_{x=u_+,y=u_-},$$
(10)

$$a_{l}(n) = \left(\frac{i}{2}\right)^{n} \frac{n_{n+2l}C_{l}}{(n+2l)4^{l}},$$
(11)

$$B_{m'}(b,c) = (-b)^{m'} \sum_{k=0}^{[m'/2]} \frac{(-c/b^2)^k}{k!(m'-2k)!},$$
 (12)

$$b_{j_1}(b) = (b/2)^{j_1}(j_1 - 1)! \sum_{k_1 = 0}^{\lfloor j_1/2 \rfloor} \frac{b^{-2k_1}}{k_1!(j_1 - k_1)!(j_1 - 2k_1 - 1)!},$$
(13)

$$c_{j_{2}}(c) = 2 \exp(c/2)(c/8)^{j_{2}}(2j_{2}-1)! \sum_{k_{2}=0}^{j_{2}-1} \times \frac{(2/c)^{k_{2}}}{k_{2}!(j_{2}-k_{2}-1)!(2j_{2}-k_{2})!},$$
 (14)

with $j_1 > 0$, $j_2 > 0$, $b_0(b) = 1$, and $c_0(c) = \exp(c/2)$. The details of the derivations of these formulas will be presented subsequently elsewhere.

To put the above analysis in a broader perspective, we discuss some related issues in the literature [2,6–8]. Keldysh [2] used the saddle point method but only included $L_C(\vec{p}, +)$. His results are different from our results by a factor of 2—i.e., $L(\vec{p}) \approx L_C(\vec{p}, +)_{Keldysh} = \frac{1}{2}L_C(\vec{p}, +)$. This is due to the fact that the saddle point method is an approximated



FIG. 2. Photoionization rates for the 1s hydrogen atom with the wavelength $\lambda = 248$ nm are plotted. The solid line stands for $W_0(L_C(\vec{p}) - L_R(\vec{p}))$, the dashed line only includes the contribution from the pole $u = u_+$ —i.e., $W_0(L_C(\vec{p}, +))$ —and the dotted line includes the contributions from two poles $u = u_{\pm}$ —i.e., $W_0(L_C(\vec{p}))$.

method while the residue theorem is the exact calculation. However, we note that if we take into account the contribution from $L_R(\vec{p})$, this accidental relation $L(\vec{p}) \approx \frac{1}{2}L_C(\vec{p})$ will not in general hold. Mishima *et al.* [6] adopted the residue theorem and obtained $L_C(\vec{p}, +)$, but they did not include $L_C(\vec{p}, -)$ and $L_R(\vec{p})$. Gribakin and Kuchiev [7] adopted the saddle point method and included $L_C(\vec{p}, +)$ and $L_C(\vec{p}, -)$. Similar to Keldysh's results, their results are also different from ours by a factor of 2. Recently, Chao [8] has pointed out that for states of general molecular systems other than the 1*s* hydrogenic state, the results obtained using the saddle point method and the residue integration method are qualitatively different.

It is instructive to compute Eqs. (8) and (9) numerically and compare the photoionization rates W_0 in Eq. (1) with and without $L_C(\vec{p}, -)$ and $L_R(\vec{p})$. We define W_0 for three cases: i.e., $L(\vec{p})=L_C(\vec{p}, +)$, $L(\vec{p})=L_C(\vec{p}, +)+L_C(\vec{p}, -)=L_C(\vec{p})$, and $L(\vec{p})=L_C(\vec{p})-L_R(\vec{p})$ as $W_0(L_C(\vec{p}, +))$, $W_0(L_C(\vec{p}))$, and $W_0(L_C(\vec{p})-L_R(\vec{p}))$, respectively, and plot them in Fig. 2 where the wavelength λ =248 nm is used. One can easily see that compared with the contributions from $L_C(\vec{p}, \pm)$, the contribution of $L_R(\vec{p})$ is almost negligibly small. Making a comparison between $W_0(L_C(\vec{p}, +))$ and $W_0(L_C(\vec{p}))$, we find that except for the intensity around 2×10^{14} W/cm², the contribution of $L_C(\vec{p}, -)$ increases the photoionization rate about twice. The main contribution results from $L_C(\vec{p}, +)$ while $L_C(\vec{p}, -)$ is almost the same order as $L_C(\vec{p}, +)$. Our numerical results suggest that even if $L_R(\vec{p})$ is omitted, the qualitative feature and the order of magnitudes will not change for the 1s hydrogen atom case. In other words, this fact may not be applicable to other atomic or even molecular systems. The contribution from $L_R(\vec{p})$ for other atomic and molecule systems will be examined in our subsequent works. To sum up, we believe that the present analysis completes and validates our mathematical analysis of the Keldysh integral and resolves the ambiguities mentioned in the preceding Comment.

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