Generalized Momentum of Tunnelling Ionization of Hydrogenic Atom in Linearly Polarized Laser

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Abstract— **We extend the Keldysh theory to study the characteristics of ionization rate of a hydrogenic atom subjected to intense lasers field. We obtain an exact semianalytical result of the ionization rate for the linearly polarized laser field. The Keldysh's theory is generalized for arbitrary momentum of the photoelectron. We study the contribution of an additional term, associated with the second pole neglected in Keldysh's theory, to the photoionization spectra of the exact rates as functions of frequency and electric field strength.**

I. Introduction

Tunnelling ionization is an important concept that well adapted for the contribution to the development of various pioneer researches such as ultrafast laser field and high harmonic generation [1] over the past few dacades. Among these works, high harmonic generation significantly leads to the advancement of the intense laser [2] field and attoseconds physics [3], [4]. Earlier important works on electron dynamics [5] such as Smirnov and Chibisov [6] provides a theoretical framework to describe the breaking up of atomic particles when the atom was placed in an homogeneous electric field but the result is concerned on the probability of the detachment of an electron per unit time. Meanwhile, Keldysh's [7] theory was high-lighted among some earlier works for providing a complete model on the theoretical description on the tunnel- and auto-ionization of the atom in an intense laser field. The laser field applied on the atom is linearly polarized and the photon energy is lower than the ionization potential. However, the model describes another important phenomenon which is the multi-photon ionization when the photon energy higher than the ionization potential of the atom. This phenomenon is prominent on describing the absorption of several N_m quanta during the transition of the electron of the bound state to free state. In Keldysh's model, the adiabatically parameter γ [8], [9], [10] shows the ratio of the tunnelling frequency to the laser frequency which is significantly describing an electron tunnels through a barrier created by an electric field of the laser. Besides, this parameter is important to determine whether the photoionization is in tunnelling or multiphoton region.

Extension on photoionization as in the well known ADK [11] (Ammosov, Delone and Krainov) theory that expressed the probability of tunnelling ionization in an alternating field, of a complex atom and of an atomic ion that are in arbitrary state based on the result of Perelomov, Popov and Terent'ev [12]. Their work is using the generalized asymptotic wavefunction and obtain the final photo-ionization rate for any arbitrary values of l in an electric field of arbitrary ellipticity, where l is the azimuthal quantum number. The calculation of the atomic ionization rate is reduced to averaging the rate in a constant field over a period of the external field in the low-frequency limit case of an alternating electromagnetic field, namely $\omega \ll \omega_t$, and where $\omega_t = 1/\tau_t$ and where τ_t is the tunnelling time as in mentioned in Keldysh work. Furthermore, extension on the tunnelling ionization concept by P. B. Corkum [13] on the classical description of the electron dynamics which is known as the "simple man model". This model describes electron in the strong electromagnetic field, tunnel to the continuum and recollide with the parent ion thus providing the basis of the high harmonic generation. As a result of the recollison, the photon is emitted resulting in the maximum energy, $N_m\hbar\omega_0 = I_p + 3.17U_p$, where N_m is the number of incident photon, $\hbar$ is the reduced Planck's constant, I_p is the ionization potential energy and $U_p = E_0^2/4m_e\omega_0^2$ is the ponderomotive energy, E_0 is the electric field, m_e is the mass of electron and ω_0 the photon angular frequency. Further extension in the past decade by M. Lein incorporates recolliding electrons for molecular imaging [14], [15] and thus providing the important foundations leading to the development of the intense light matter interactions [16], [17].

Recently, various experimental works lead to the generation of high-energy attosecond light sources [18] from gas based on the extension of the concept of tunnelling ionization. The theory of high-harmonics generation where the electron under the influence of the electric field is driven to the continuum state which is described by Volkov wavefunction, then returns and recollide to the parent ion [19], and thus emitting a plateau of harmonics where the cutoff is located at $I_p + 3.17U_p$. This phenomenon is the main source of producing the attosecond light. The nature of the cutoff and whether any other possible value beside $I_p + 3.17U_p$ is still remain a mystery and vast number of works and researches still trying to figure out the reason. Meanwhile, D. B. Milošević and A. F. Starace [20] had showed that the linearly polarized laser with the static field perpendicular to the laser field can induce a plateau towards high energy X-ray photons. K. J. Yuan and A. D. Bandrauk [21],[22] in their recent works show that the high harmonic generation is not limited to the recollision of the electron with parent ion. For the molecules case, the recollision of electron with the neighbouring ion can produce the high harmonic generation as well. They had performed numerical results that showed the molecular high-order harmonic generation can

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have the maximum elliptically polarized harmonic energies of $I_p + 13.5U_p$ [23] for certain internuclear distances and also relative pulse carrier envelope phase. Progress in ultrashort-pulse lasers has provided the capability of attaining high enough laser intensities that it is possible to observe tunnel ionization in the near infrared spectral range, before the ionization process reaches saturation.

In this paper, we have extended the Keldysh theory to study the characteristics of ionization rate of a hydrogenic atom subjected to linear polarized intense lasers field. An exact semianalytical result was obtained for the ionization rate of the photoelectron in z-direction. We generalized the semianalytical result so that it can adapt arbitrary momentum of the photoelectron through the tunnelling ionization. We found an additional term that associated with the second pole which is neglected in Keldysh's theory. The exact tunnelling ionization rate of photoelectron is plotted as functions of frequency and electric field strength.

II. Keldysh Theory for Linear Polarized Laser Field

In our calculation, we derive the Volkov wavefunction that describe the wavefunction of an electron in external electric field of

$$\mathbf{E}(\mathbf{t}) = \mathbf{E}\cos\omega t \quad (1)$$

The Volkov wavefunction takes the form

$$\begin{aligned}\Psi(\mathbf{r},t) &= \exp\left(\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}\right)\times \\ &\exp\left\{-\frac{i}{\hbar}\left[\frac{1}{2m}\int_0^t\left(p+\frac{eE_0}{\omega}\sin\omega\tau\right)^2 d\tau\right]\right\}\end{aligned} \quad (2)$$

After doing length gauge transformation on (2), the final form takes

$$\Psi_p(\mathbf{r},t) = \exp\left\{\frac{i}{\hbar}\left\{\mathbf{\Pi}(t)\cdot\mathbf{r} - \left[\frac{1}{2m}\int_0^t \mathbf{\Pi}(t)^2 d\tau\right]\right\}\right\} \quad (3)$$

where

$$\Pi(t) = \mathbf{p} - e\mathbf{A}$$

and $\mathbf{A} = \frac{e\mathbf{E}}{\omega}\sin\omega t$ is the vector potential.

Next, we use the hydrogen s-th bound state at $n=1$, $l=0$ and $m=0$ as the initial state for the tunnelling ionization

$$\begin{aligned}\psi(\mathbf{r}) &\to \psi_{100}(\mathbf{r},\theta,\phi) \\ &= \left(\frac{1}{\pi a^3}\right)\exp\left(-\frac{\mathbf{r}}{a}\right)\end{aligned} \quad (4)$$

where $a = a_0/Z$

For the transition matrix, we have

$$V_{0s}(\mathbf{p},t) = \int \Psi_p^*(\mathbf{r},t)\, e\mathbf{E}(\mathbf{r},t)\cdot\mathbf{r}\Psi_s(\mathbf{r},t)\, d^3r \quad (5)$$

$\mathbf{r}$-vector take $r(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, since our case is for linearly polarized laser field, hence we choose the propagation is along the z-direction.

We separate (5) into two part, the matrix element prefactor (spatial part) and also the action part (time dependent part).

The matrix element prefactor

$$\begin{aligned}V_0(\mathbf{\Pi}(t)) &= \left(\frac{1}{\pi a^3}\right)^{\frac{1}{2}}\times \\ &\int\exp\left[-\frac{i}{\hbar}\mathbf{\Pi}(t)\cdot\mathbf{r}\right] e\mathbf{E}\cdot\mathbf{r}\exp\left(-\frac{\mathbf{r}}{a}\right)d^3r\end{aligned} \quad (6)$$

The action part

$$\begin{aligned}e^{iS(\mathbf{p},t)} &= e^{i\Omega(p)t}\times \\ &\exp\left\{-\frac{i}{\hbar}\left[\frac{e\mathbf{p}\cdot\mathbf{E}}{m\omega}(\cos\omega t - 1) + \frac{e^2\mathbf{E}^2}{8m\omega^2}\sin 2\omega t\right]\right\}\end{aligned} \quad (7)$$

where

$$\begin{aligned}\Omega(p) &= \frac{1}{\hbar}\left(I_0 + \frac{p^2}{2m} + \frac{e^2E^2}{4m\omega^2}\right) \\ &= \frac{1}{\hbar}(I_0 + K + U_p)\end{aligned} \quad (8)$$

Next, we solve for the matrix element prefactor. By using the transformation $u = \sin\omega t$, the result yields

$$V_0\left(\mathbf{p}+\frac{e\mathbf{E}}{\omega}u\right) = -i\frac{2\pi}{\hbar}\sqrt{\frac{1}{\pi a^3}}e16a^5I_0^3\frac{\mathbf{E}\cdot\left(\mathbf{p}+\frac{e\mathbf{E}}{\omega}u\right)}{\left[\frac{\hbar^2}{2ma^2}+\frac{\left(\mathbf{p}+\frac{e\mathbf{E}}{\omega}u\right)^2}{2m}\right]^3} \quad (9)$$

Meanwhile, for the action part, we set

$$\widetilde{I_0} = I_0 + U_p \quad (10)$$

hence,

$$\begin{aligned}S(\mathbf{p},t) &= \frac{1}{\hbar}\left[\left(\widetilde{I_0}+\frac{p^2}{2m}\right)t - \frac{e\mathbf{p}\cdot\mathbf{E}}{m\omega}(\cos\omega t - 1)\right. \\ &\left.-\frac{e^2\mathbf{E}^2}{8m\omega^2}\sin 2\omega t\right]\end{aligned} \quad (11)$$

We perform the same transformation as in matrix element prefactor, (11) can bee expressed as

$$\begin{aligned}S(\mathbf{p},u) &= \frac{1}{\hbar\omega}\left[\left(\widetilde{I_0}+\frac{p^2}{2m}\right)\sin^{-1}u\right. \\ &\left.-\frac{e\mathbf{p}\cdot\mathbf{E}}{m\omega}\left(\sqrt{1-u^2}-1\right) - \frac{e^2\mathbf{E}^2}{8m\omega^2}u\sqrt{1-u^2}\right] \\ &= N\sin^{-1}u - a\left(\sqrt{1-u^2}-1\right) - bu\sqrt{1-u^2}\end{aligned} \quad (12)$$

where

$$N = \frac{\widetilde{I}_0}{\hbar\omega} + \frac{\chi^2 I_0}{\hbar\omega} = \frac{\widetilde{I}_0}{\hbar\omega} + 2\gamma^2\chi^2 b \quad (13)$$

$$a = \frac{1}{\hbar\omega}\frac{e\mathbf{p}\cdot\mathbf{E}}{m\omega} = \frac{2I_0}{\gamma\hbar\omega}\xi\chi = (4b\gamma)\,\xi\chi \quad (14)$$

$$b = \frac{1}{\hbar\omega}\frac{e^2\mathbf{E}^2}{8m\omega^2} = \frac{U_p}{\hbar\omega} \quad (15)$$

$$\xi = \cos\theta \quad (16)$$

The momentum depends on n through

$$\chi = \frac{p_n}{\sqrt{2mI_0}} = \sqrt{\frac{\hbar\omega}{I_0}(n-n_0)}, \quad (17)$$

where $n_0 = \frac{I_0+U_p}{\hbar\omega}$ and $p_n = \sqrt{2m\hbar\omega(n-n_0)}$.

For linearly polarized, the ionization rate is for small momentum was first derived by Keldysh in Ref. [7]. The theory is valid for small momenta such that terms higher than $(\frac{p}{\sqrt{2mI_0}})^2$ are negligible. This restriction also implies a limitation to the laser field E (since $\frac{d\mathbf{p}}{dt} \simeq e\mathbf{E}$) and hence the Keldysh parameter γ.

The Keldysh parameter has the alternative statements,

$$\gamma = \sqrt{\frac{E_B}{2U_p}} = \frac{\omega}{I^{1/2}}\sqrt{2E_B} = \sqrt{\frac{I_0}{2U_p}} \quad (18)$$

where E_B is the field free binding energy of the electron in the atom or I_0 the ionization potential of the atom.

U_p is the ponderomotive energy (the interaction energy during the transition) of the free electron in the field, and ω is the frequency of the ionization field of intensity I.

We combine the matrix element prefactor and the action and rewrite it in the form

$$L(\mathbf{p}) = \frac{1}{2\pi}\oint V_0\left(\mathbf{p} + \frac{e\mathbf{E}}{\omega}u\right)\exp\left\{\frac{i}{\hbar\omega}\int_0^u I_0 + \frac{1}{2m}\right\} \quad (19)$$

Next, we apply Saddle point method on (19),

$$\frac{dS(\mathbf{p},t)}{dt} = \frac{1}{\hbar}\left[I_0 + \frac{1}{2m}\left(\mathbf{p} + \frac{e\mathbf{E}}{\omega}\sin\omega t\right)^2\right] = 0 \quad (20)$$

Two saddle point are obtain from (20)

$$u_\pm = \frac{1}{4b}\left[-a \pm \sqrt{(a^2 - 8bN + 8b^2)}\right] = -y \pm \sqrt{y^2 + \frac{b-N}{2b}} \approx \gamma\left[-x\cos\theta \pm i\left(1 + x^2\frac{1}{2}\sin^2\theta\right)\right] \quad (21)$$

$$u_- = u_+^* \quad (22)$$

The second order of the action part becomes

$$S''(u) = \frac{\frac{e}{m\omega}\mathbf{E}\cdot\left(\mathbf{p} + \frac{e\mathbf{E}}{\omega}u\right)}{\hbar\omega\sqrt{1-u^2}} + \frac{u\left[I + \frac{1}{2m}\left(\mathbf{p} + \frac{e\mathbf{E}}{\omega}u\right)^2\right]}{(1-u^2)^{3/2}} \quad (23)$$

Hence,

$$S''(u_s) = \frac{\frac{e}{m\omega}\mathbf{E}\cdot\left(\mathbf{p} + \frac{e\mathbf{E}}{\omega}u_s\right)}{\hbar\omega\sqrt{1-u_s^2}} = \pm 4\frac{U_p}{\hbar\omega}\frac{i\gamma\sqrt{1+\chi^2 s^2}}{\sqrt{1-u_\pm^2}} = \pm\frac{2U_p}{\hbar\omega}\frac{u_+ - u_-}{\sqrt{1-u_\pm^2}} \quad (24)$$

Next, we rewrite again for the $L(\mathbf{p})$ function

$$L(\mathbf{p}) = \frac{16ieI_0^3\sqrt{\pi a^7}}{\hbar^2\omega}\sum_s \frac{\mathbf{E}\cdot\left(\mathbf{p} + \frac{e\mathbf{E}}{\omega}u_s\right)}{(\hbar\omega)^2 S''(u_s)^2\left(\sqrt{1-u_s^2}\right)^3} e^{iS(\mathbf{p},u_s)} = \frac{4\hbar\omega I_0\sqrt{\pi a}}{eE}\sum_{s=\pm}\frac{e^{iS(\mathbf{p},u_s)}}{\cos\Theta^s\cos\omega t_s} \quad (25)$$

A. Rate for small momentum

The celebrated formula for ionization rate written as

$$w = 8\omega\sqrt{\frac{2I_0}{\hbar\omega}}\xi^{3/2}\exp[2n_0(\frac{\gamma\sqrt{1+\gamma^2}}{2\gamma^2+1} - \sinh^{-1}\gamma)] \times \sum_{n=n_0}^{\infty}\exp\left[2\Delta n(\xi - \sinh^{-1}\gamma)\right]\mathcal{D}(\sqrt{2\xi\Delta n}) \quad (26)$$

where $\Delta n = n - n_0$, $\xi = \frac{\gamma}{\sqrt{1+\gamma^2}}$, $I_0 = \frac{\hbar^2}{2ma^2}$ is the ionization energy with the Bohr radius a, $U_p = \frac{e^2E^2}{4m\omega^2}$ is the ponderomotive energy, $n_0(E,\omega) = \frac{I_0+U_p}{\hbar\omega}$ with the Dawson integral

$$\mathcal{D}(y) = \int_0^y \exp(z^2 - y^2)dz \quad (27)$$

$$y^2 = 2\xi\Delta n \quad (28)$$

Equation (26) is two times larger than that in ref. [8] because the two poles are included.

B. Exact rate for arbitrary momentum

We have extended the Keldysh theory to arbitrary momenta, giving the exact result that is semi-analytical,

$$w = \frac{m}{(2\pi\hbar^2)^2}2\pi\int_0^\pi\sum_{n=n_0}^{\infty}|L(\mathbf{p}_n)|^2 p_n\sin\Theta d\Theta \quad (29)$$

where

$$|L(\mathbf{p}_n)|^2 = (\frac{4\hbar\omega I_0}{eE})^2\pi a\left|\frac{e^{iS(\mathbf{p}_n,u_+)}}{\eta_+\cos\omega t_+} + \frac{e^{iS(\mathbf{p}_n,u_-)}}{\eta_-\cos\omega t_-}\right|^2 \quad (30)$$

with double saddle points

$$\eta_{\pm} = \pm\sqrt{1+\chi^2\sin^2\Theta} + i\frac{u_{\pm}^3}{\gamma} \tag{31}$$

$$u_{\pm} = -\gamma\chi a_z \pm \gamma\sqrt{(\chi a_z)^2 - (1+\chi^2)} \tag{32}$$

$$\omega t_{+} = \sin^{-1} u_{+}, \tag{33}$$

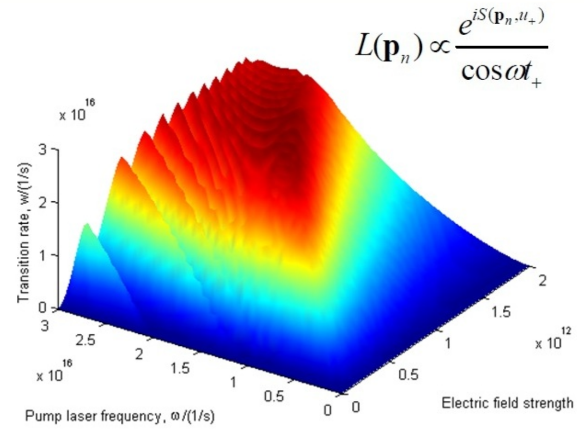
$$\omega t_{-} = \pi - \sin^{-1} u_{-} \tag{34}$$

and $a_z = \cos\Theta$.

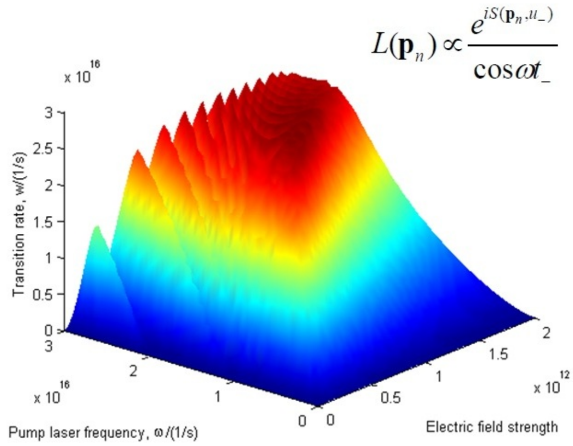
III. Results and Discussions

In Fig. 1a, we can see the rate of tunnelling ionization due to the positive pole during the saddle point calculation as in Eqn. (30). It is clearly showed that the rate increases with the frequency and electric field strength. We observe the oscillations at the frequency around 10^{16} s^{-1} with the change of electric field. Meanwhile, Fig. 1b has shown the rate of tunnelling ionization due to the negative pole. However, the oscillations pattern in Fig. 1b is almost having the same shape as in Fig. 1a. In Fig. 1c, the exact rate of the tunnelling ionization is computed by taking account of the two poles was shown as the function of frequency and electric field strength. Interesting feature was found due to the interference of the two terms $\frac{e^{iS(\mathbf{p}_n,u_+)}}{\cos\omega t_+}$ and $\frac{e^{iS(\mathbf{p}_n,u_-)}}{\cos\omega t_-}$ in Eqn. (30) associated with the two saddle points $u_{\pm}$. The inteference in Fig. 1c has a increment of a ratio $2\sqrt{pi/2}$ which is obviously as a result of Eqn. (25) and Eqn. (30). These multiple poles mainly contribute after taking the consideration of higher order term of momentum in our calculation meanwhile in Keldysh's original work, small momentum approximation was taken for the elimination of higher order momentum term in order to simplify the calculation. In our understanding, for the first time this interference pattern predominantly appears in the tunnelling ionization rate of photoelectron. Therefore, it would be interesting and also challenging for the further experimental verification. Consequently, our result can take arbitrary value of momentum into account to produce a more accurate photoionization rate.

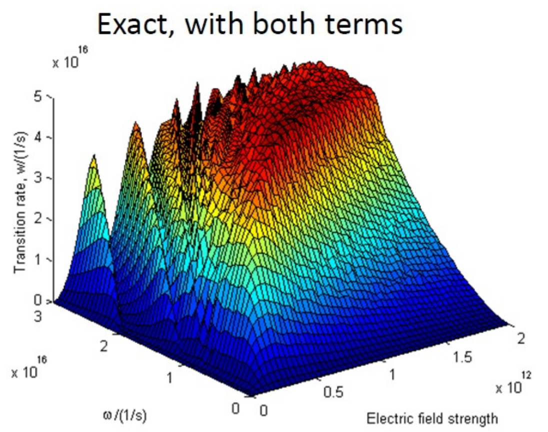
In conclusion, we have obtained an exact semi-analytical expression for the tunnelling ionization rate for the linearly polarized laser field for arbitrary momentum of the photoelectron. We found the interference pattern in the tunnel ionization rate due to the multiple poles in the saddle point calculation. Further extension can be done on this theory such as second order perturbation formalism to acquire the high harmonic generation and the effects of recollision.



(a)



(b)



(c)

Fig. 1: Ionization rate versus frequency, ω and electric field, E for (a) positive pole, (b) negative pole, and (c) both poles included.

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