

LUDWIG-MAXIMILIANS-UNIVERSITÄT  
MÜNCHEN

Bachelors Thesis

# The role of excited atomic states in multiphoton ionization

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March 29, 2025

## **Abstract**

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# 1. Introduction

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## 2. Theory

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$$\partial_t u = \mathcal{H}(t)\lambda \quad (2.1)$$

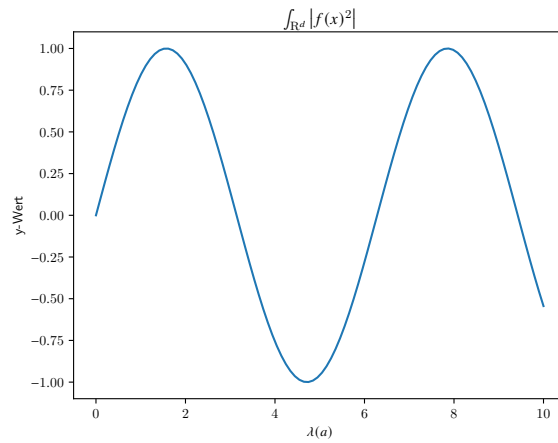


Figure 2.1: Sine function

## 2.1 Basic Formalism

### 2.1.1 schrödinger equation

Basic Definitions of schrödinger eq, light dyson series, and strong field s matrix

We want the time evolution of a quantum system in the presence of an external time dependent field in order to describe the strong field ionization later on. The time evolution of a quantum system is given by the time dependent Schrödinger equation and a general hamiltonian

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle. \quad (2.2)$$

The formal solution depends on the time dependence of the hamiltonian and the physical setting. In the following we assume <sup>1</sup> (IMPORTANT) that  $[\hat{H}(t), \hat{H}(t')] = 0$  so we assume some sort of quasi static approximation to the Hamiltons time evolution. The solution is then given by

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}(t') dt'} |\Psi(t=0)\rangle \quad (2.3)$$

Now its time so establish a physical setting. We have Hydrogen Atom with nucleus and electron described by time indepentent Hamilton  $\hat{H}_0$ . The external laser Field is descirbed by an time dependent part  $\hat{V}(t)$ . To describe the interaction of the atom with the laser field we use in the following the dipole approximation.

---

<sup>1</sup>How? Later. No physical setting bzw no approximations yet. Its better to juistify it later but have a working formalism instead of the other way around.

### 2.1.2 Light-Matter Interaction

A light wave is defined by the Maxwell equations

$$\begin{aligned}\nabla \cdot \mathbf{E}(t) &= \rho & \nabla \times \mathbf{E}(t) &= -\frac{\partial \mathbf{B}(t)}{\partial t} \\ \nabla \cdot \mathbf{B}(t) &= 0 & \nabla \times \mathbf{B}(t) &= \mathbf{J} + \frac{\partial \mathbf{E}(t)}{\partial t}\end{aligned}$$

The Maxwell equations are being solved by

$$\begin{aligned}\mathbf{E}(t) &= -\nabla\varphi(t) - \frac{\partial \mathbf{A}(t)}{\partial t} \\ \mathbf{B}(t) &= \nabla \times \mathbf{A}(t)\end{aligned}$$

For these solutions we introduced the vector potential  $\mathbf{A}(t)$  and the scalar potential  $\varphi(t)$ . These are not unique such that different choices can result in the same physical setting. In general

$$\begin{aligned}\mathbf{A}(t) &\rightarrow \mathbf{A}(t) + \nabla\chi(t) \\ \varphi(t) &\rightarrow \varphi(t) - \frac{\partial}{\partial t}\chi(t)\end{aligned}$$

also fulfill the Maxwell equations while  $\chi(t)$  is an arbitrary smooth function. The arbitrariness of  $\chi$  is known as gauge freedom and a direct consequence of the Maxwell equations. Choosing a gauge (i.e., a specific  $\chi$ ) is a matter of convenience and can be used to simplify the calculations as presented in the following.

### 2.1.3 Dipole Approximation

Very important approximation. Making it implies that

$$\mathbf{A}(\mathbf{x}, t) \approx \mathbf{A}(t) \quad \text{and} \quad \mathbf{B} = \nabla \times \mathbf{A} \approx 0 \quad (2.4)$$

Therefore we can rewrite the time dependent part  $\hat{V}$  of our Hamiltonian as

$$\hat{V}(t) = -\hat{\mathbf{d}} \cdot \mathbf{E}(t) \quad (2.5)$$

where  $\hat{\mathbf{d}}$  is the dipole operator and  $\mathbf{E}(t)$  is the electric field.



## 2.2 Strong Field Approximation

For making the strong field approximation we first have to obtain a point where it is good to use. When we treat  $\hat{V}(t)$  as the interaction term, we can write an exact solution to (2.2)

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}(t') dt'} |\Psi(t=0)\rangle + \int_{t_0}^t dt' e^{-\frac{i}{\hbar} \int_{t'}^t \hat{H}(t'') dt''} \hat{V}(t') e^{-\frac{i}{\hbar} \int_{t_0}^{t'} \hat{H}(t'') dt''} |\Psi(t=0)\rangle \quad (2.6)$$

## 2.3 Strong Field Ionization

Derivation of

$$\lim_{t \rightarrow \infty} |\Psi(t)\rangle = -i \int d^3p |\mathbf{p}\rangle \int_{-\infty}^{\infty} dt' e^{-\frac{i}{2} \int_{t'}^{\infty} [\mathbf{p} + \mathbf{A}(t')]^2 dt'} e^{iI_{\mathbf{p}} t'} \langle \mathbf{p} + \mathbf{A}(t') | \hat{\mathbf{d}} \cdot \mathbf{E}(t') | \Psi_0 \rangle \quad (2.7)$$

## 2.4 Multiphoton Ionization

Different types of Ionization, tunneling Ionization, multiphoton

## 3. Numerical Methods

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### 3.1 tRecX

## 3.2 Python Ionization Model

## 4. Results and Discussion

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$$\partial \mathbf{A} = \mathfrak{B}$$

$$\int_{\mathbb{R}^d} |f(x)|^2 dx = \int_{\mathbb{R}^d} |\mathcal{F}f(\xi)|^2 d\xi \quad (4.1)$$

$$i\partial_t u = \mathcal{H}(t) |a\rangle \lambda \quad (4.2)$$

for this calculation [1] was used

### 4.1 Laser Fields

## 5. Conclusion and Outlook

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# A. Appendix A

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