

COMPLEX-ROTATION AND WAVE-PACKET CALCULATIONS OF THE IONIZATION RATE FOR HYDROGEN ATOM IN ELECTRIC FIELD

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Abstract. Applying two different methods, the complex rotation and the wave packet propagation method, the position and width of the lowest (resonant) state of hydrogen atom in external electric field are calculated for different field strengths. Using these results the validity of Landau formula for ionization rate in the tunneling regime is demonstrated.

1. INTRODUCTION

Ionization of the hydrogen atom in external electric field is a problem which is many times considered using different theoretical methods. Since the Hamiltonian of the system (here we use the atomic units)

$$H = \frac{p^2}{2} - \frac{1}{r} - Fz, \quad (1)$$

is separable in parabolic coordinates, for small values of the strength of electric field F it was possible to obtain approximate analytical expressions for the energy levels as functions of F , as well as the ionization rates when the atom is in the ground state (the so-called Landau formula) [1]

$$w = \frac{4}{F} \exp\left(-\frac{2}{3F}\right). \quad (2)$$

The latest expression essentially determines the probability (per unit time) of the ionization of a hydrogen atom in an electric field due to the electron tunneling through the potential barrier formed by the nuclear Coulomb potential and the constant external field (see Figure 1). A consequence of the presence of this finite barrier is that all states of the system described by Hamiltonian (1) have in fact the resonant character and formula (2) also determines the width of the lowest state.

Even today the hydrogen atom in constant electric field is frequently used as a good example for testing new theories and methods treating the problems with a perturbation which makes the spectrum continuous. Finally, within the so-called static field approximation this problem may be the first step in the analysis of ionization of atoms due to the absorption of electromagnetic radiation. Here we analyze the lowest state of the system described by Hamiltonian (1) by the use of two different methods: the complex rotation method and the wave packet propagation method.

2. COMPLEX ROTATION METHOD

A resonant state $\psi(\mathbf{r})$ can be regarded as an extension of the concept of bound state in a sense that it is an eigensolution of the Schrödinger equation which asymptotically behaves as a purely outgoing wave ($\psi(\mathbf{r})$ is not square integrable, see Figure 1) with complex eigenenergy E_{res} . The real and imaginary parts of E_{res} determine the energy (position) and the width of resonance, $E = \text{Re}(E_{\text{res}})$, $\Gamma = -2 \text{Im}(E_{\text{res}})$. The basic idea of the complex rotation method (see e.g. Ref. [2]) is to make the resonance wave function $\psi(\mathbf{r})$ square integrable by a complex rotation of the coordinate, $\psi(\mathbf{r}) \rightarrow \psi_{\theta}(\mathbf{r}) = \psi(e^{i\theta} \mathbf{r})$, where θ is a real parameter called the ‘rotation angle’. Such a ‘rotated’ state $\psi_{\theta}(\mathbf{r})$ is an eigenfunction of the so-called complex rotated Hamiltonian H_{θ} obtained from the original Hamiltonian H by the transformations $\mathbf{r} \rightarrow e^{i\theta} \mathbf{r}$, $\mathbf{p} \rightarrow e^{-i\theta} \mathbf{p}$. The spectrum of Hamiltonian (1) can be computed by diagonalizing the corresponding rotated Hamiltonian in a square integrable basis which is complete in a sense that it covers the continuous part of the spectrum, too. For this purpose we have used here the Sturmian basis [3]. Some results are shown in Table 1 as well as in Figure 2.

3. WAVE PACKET APPROACH

Alternatively the resonant states can be studied using a time dependent approach. If $\psi(\mathbf{r},0)$ is an initial wave function (wave packet) one can calculate the wave function $\psi(\mathbf{r},t)$ at an arbitrary time t by integrating the time dependent Schrödinger equation. Technically, this method reduces to the construction of a sufficiently accurate representation for the evolution operator $U(\Delta t)$, where Δt is a small time step. Then, the wave function $\psi(\mathbf{r},t)$ at a discretized time t can be obtained by integrating numerically the relation $\psi(\mathbf{r},t + \Delta t) = U(\Delta t)\psi(\mathbf{r},t)$. The energy spectrum for a given system can be obtained from the autocorrelation function $c(t)$, which is the overlap between the functions $\psi(\mathbf{r},t)$ and $\psi(\mathbf{r},0)$, by calculating its power spectrum (i.e. $|\text{FT}[c(t)]|^2$, where $\text{FT}[c(t)]$ is the Fourier transform of $c(t)$). In the power spectrum resonances appear as (approximate) Lorentzian profiles containing the information about their positions (E) and widths (Γ). In order to calculate E and Γ for the lowest state of the system determined by Hamiltonian (1), we choose for $\psi(\mathbf{r},0)$ to be the unperturbed ground state wave function of the hydrogen atom and calculate its evolution by the use of a variant of the second-order-differential scheme [4]. Since $\psi(\mathbf{r},0)$ for

$F > 0$ is not a stationary state, initially it moves periodically as a wave-packet in the potential $V = -1/r - Fz$. However, at each reflection from the potential barrier a part of the packet transmits in the outer region, and after some time (~ 100 a.u.) it reduces to an almost stationary state with well defined outgoing wave – the resonance wave function ψ (see the top of Figure 1).

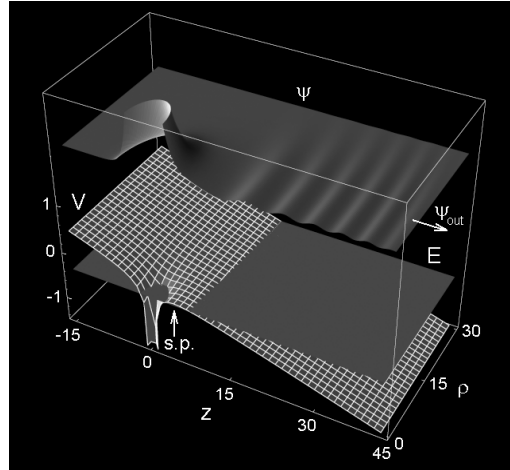


Figure 1. Bottom: The potential $V = -1/r - Fz$ (in cylindrical coordinates) for the field strength $F = 0.05$ a.u. and the corresponding lowest energy level E . The vertical arrow shows the position of the saddle point (s.p.) of the potential barrier. Top: The real part of the total wave function ψ corresponding to the lowest level.

4. RESULTS

Table 1. The positions E and widths Γ of the lowest energy level of hydrogen atom in external electric field for different field strengths F (all in atomic units) obtained using the complex rotation (CR) and the wave packet (WP) methods.

F	E (CR)	Γ (CR)	E (WP)	Γ (WP)
0	-0.5	0	-0.5	0
0.05	-0.5061	0.772E-4	-0.5061	0.66E-4
0.10	-0.5274	0.01453	-0.5276	0.01405
0.15	-0.5511	0.06004	-0.5514	0.05878
0.20	-0.5701	0.1212	-0.5694	0.1212
0.25	-0.5850	0.1895	-0.586	0.192

The values for the energy (position) E and width Γ of the lowest state at several strengths of electric field are shown in Table 1. The results obtained by the two methods are mutually in a good agreement and also in agreement with results of other authors [5]. Generally, the complex rotation method produces the

results with higher accuracy, but the time dependent method gives a better insight into dynamics of the ionization process. Roughly speaking, this process, depending on the field strength, realizes either as the tunnel ionization if $E < V_{\text{sp}}$ or as the over-barrier ionization if $E > V_{\text{sp}}$. V_{sp} is the value of the potential V at the saddle point of potential barrier (see Figure 1). It is found that $E = V_{\text{sp}}$ for $F \approx 0.065$ a.u. Finally, we have compared the numerically obtained results with Landau formula (2) (with the assumption that $w = \Gamma$) and confirmed that the formula is valid in the regime of tunnel ionization (see Figure 2).

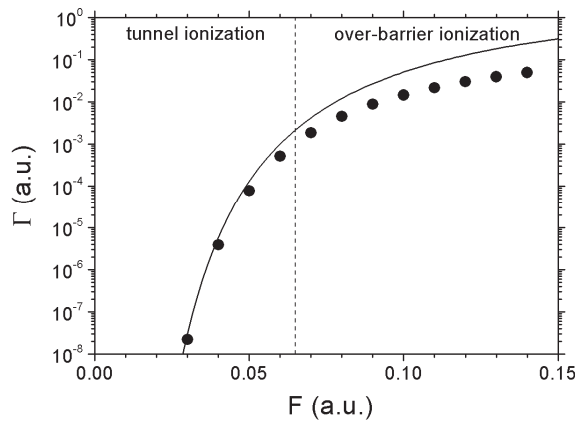


Figure 2. The comparison between numerical data (complex rotation method) for the width Γ of the lowest energy level of hydrogen atom in external electric field F (circles) and the formula (2) for the ionization rate w (full line). The vertical dashed line denotes the value of the field ($F \approx 0.065$ a.u.) when the lowest energy level is equal to the saddle point of the potential barrier.

Acknowledgements

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