Population coherent control of a Rydberg sodium atom in a microwave field*

Jiang Li-Juan(蒋利娟)[a)b)†], Zhang Xian-Zhou(张现周)[a)‡], Jia Guang-Rui(贾光瑞)[a)], Zhang Yong-Hui(张永慧)[a)], and Xia Li-Hua(夏立华)[a)]

[a)] *Department of Physics, Henan Normal University, Xinxiang* 453007, *China*
[b)] *Department of Physics, Xinxiang University, Xinxiang* 453000, *China*

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The B-spline expansion technique and the time-dependent multilevel approach (TDMA) are used to study the interaction between a microwave field and sodium atoms. The Rydberg sodium atom energy levels of p states in zero field are calculated, and the results are in good agreement with the other theoretical ones. The time evolutions during the population transfers of the five states from $n = 75$ to $n = 79$ in different microwave fields are obtained. The results show that the coherent control of the population transfer from the lower states to the higher ones can be accomplished by optimizing the microwave pulse parameters.

Keywords: B-spline, population transfer, multilevel system

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1. Introduction

The coherent transfer of atomic population into a given quantum state is an important problem to be addressed in a variety of fields of contemporary science and technology.[1−3] The adiabatic rapid passage (ARP) is an approximately 100% efficient way to transfer the population from one state to another. The high efficiency of each step allows the population to be transferred through many levels by sequential ARPs, which can make the population transfer possible by using a coherent chirped radiation field. This unique character makes it quite attractive in atomic physics and chemistry.

The development of tunable dye lasers allows excited high Rydberg n, l states in atoms to reach an efficient population. This fact has brought about a renewed interest to the experimental and the theoretical studies in this field. A number of studies concerning highly excited states of different atoms, such as Na,[4,5] Li,[6] K,[7,8] Sr,[9] Ba,[10,11] He,[12] and Xe,[13] have become the hot subjects in the last few decades. Meerson and Friedlang[14] suggested that using a microwave pulse initially at the Kepler frequency and chirped to a lower frequency would transfer atoms to a higher n state, leading to the ionization at a lower microwave field. Bensky *et al.*[15] and Wesdorp *et al.*[16] suggested that it might be more interesting to chirp the frequency in the other direction; they demonstrated that it was possible to induce the electron–ion recombination into high-lying Rydberg states with half cycle pulses, and the technique could be a way to produce antihydrogen.[17] Recently, the coherent population transfer of Rydberg atoms induced by the frequency- or amplitude-chirped pulses has also been used to carry out quantum control of physical and chemical processes by using the robustly driving transitions between quantum states.[18,19] The result shows that the population transition probability is sensitive to the laser pulse parameters and the chirped rate, so it is important to choose suitable laser pulse parameters to enhance the population transition probability. In this paper, we numerically investigate the population transfers of Rydberg sodium atoms with $n = 75$ to 79 ($l = 0$, 1 for a given n) by exposing them to specially designed laser pulses. We achieve as complete as possible population transfer between the selected states of the sodium atoms by optimizing the

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†Corresponding author. E-mail: jianglijuan2003@163.com
‡Corresponding author. E-mail: xz-zhang@henannu.edu.cn

microwave pulse parameters.

2. Theory

We consider a sodium atom in a microwave field $E(t)$ (the direction of field is along the z axis). The time-dependent Schrödinger equation for the outer electron of the atom takes the form (in atomic units)

$$\mathrm{i}\frac{\partial\psi(\boldsymbol{r},t)}{\partial t} = H\psi(\boldsymbol{r},t), \tag{1}$$

where $H = H_0 + zE(t)$ is the Hamiltonian of the system under consideration, $H_0 = p^2/2 + V(r)$ is the zero-field Hamiltonian, and $E(t) = E_0 f(t)\cos\omega t$ is the driving microwave pulse. Here E_0 is the amplitude of the microwave field, $f(t)$ describes the shape of the microwave field

$$f(t) = \begin{cases} \sin^2\left(\dfrac{\pi t}{mT}\right)\sin\omega t, & 0 \le t \le mT, \\ \sin\omega t, & t \ge mT, \end{cases} \tag{2}$$

with $\omega = \omega_0 + \beta t$, ω_0 the laser initial frequency, β the chirped rate, T the microwave pulse period, and m the number of the microwave pulse period. Using the B-spline basis function and the one-electron model potential,[20] we obtain the eigenfunctions of H_0 by solving the stationary Schrödinger equation. Then choosing eigenfunctions of H_0 as the basis, we solve the time-dependent Schrödinger equation using the time-dependent multilevel approach (TDMA) and obtain the transition probability of the sodium atoms.

2.1. *B*-spline and model potential

B-splines are piecewise polynomials, which possess the characteristics of both analytical and numerical functions and are thus a very important tool for numerical calculations.[21–23] Given a knot sequence on the z axis, $\{a = t_1 \le t_2 \le t_s \cdots \le t_{n+k} = b\}$, B-spline functions of order k are defined as[21]

$$\begin{aligned} B_{i,l}(x) &= \begin{cases} = 1, \ t_i \le x \le t_{i+1}, \\ = 0, \ \text{otherwise}, \end{cases} \\ B_{i,k}(x) &= \frac{x - t_i}{t_{i+k-1} - t_i} B_{i,k-1}(x) \\ &\quad + \frac{t_{i+k} - x}{t_{i+k} - t_{i+1}} B_{i+1,k-1}(x). \end{aligned} \tag{3}$$

It is immediately seen that $B_{i,k}$ is a piecewise polynomial of order $k-1$ localized within $[a, b]$, while $B_{i,k}$ is nonvanishing within $[t_i, t_{i+k}]$. The behaviors of the B-spline functions can be readily adjusted with the knot sequence, viz., the choices of knot point t_i, order k, and number of B-splines N, which offers means to optimize the B-spline basis set to expand the wavefunctions.

The one-electron model potential given by Schweizer *et al.*[20] can well describe the motion of the valence electron of the alkali-metal atom. The form of this potential is

$$\begin{aligned} V &= -\frac{1}{r}[\tilde{Z} + (Z - \tilde{Z})\exp(-a_1 r) \\ &\quad + a_2 r\exp(-a_3 r)], \end{aligned} \tag{4}$$

where a_1, a_2, and a_3 are the parameters, which have been given in Ref. [20], and Z is the nuclear charge of the neutral atom. For the sodium atom, $Z = 11$, $\tilde{Z} = 1$, $a_1 = 7.902$, $a_2 = 23.51$, and $a_3 = 2.688$. Thus, the model potential of the sodium atom becomes

$$\begin{aligned} V(r) &= -\frac{1}{r}[(11-1)\exp(-7.902r) \\ &\quad + 23.51r\exp(-2.688r) + 1]. \end{aligned} \tag{5}$$

2.2. Solution of the stationary Schrödinger equation

Due to the central symmetry of the potential, the eigenfunction of H_0 has the following form:

$$\psi_{nlm}(r,\theta,\phi) = \frac{U_{nl}(r)}{r}\mathrm{Y}_{lm}(\theta,\phi), \tag{6}$$

where n, l, and m are principal, angular momentum, and magnetic quantum numbers, respectively, and $\mathrm{Y}_{lm}(\theta,\phi)$ is a spherical harmonic function. The radial wavefunction $U_{nl}(r)$ can be expanded into a linear combination of B-splines

$$U_{nl}(r) = \sum_{i=1}^{N} c_i B_{i,k}(r). \tag{7}$$

By substituting $U_{nl}(r)$ and $V(r)$ into the radial Schrödinger equation

$$\left[-\frac{\mathrm{d}^2}{2\mathrm{d}r^2} + \frac{l(l+1)}{2r^2} + V(r)\right]U_{nl}(r) = E_{nl}U_{nl}(r) \tag{8}$$

and then projecting on $B_{i,k}(r)$, we obtain a matrix equation

$$\boldsymbol{H}_l\boldsymbol{C} = \boldsymbol{E}\boldsymbol{S}\boldsymbol{C}, \tag{9}$$

where $\boldsymbol{H}_l$ is the Hamiltonian matrix, $\boldsymbol{S}$ is the overlap matrix, $\boldsymbol{E}$ and $\boldsymbol{C}$ are eigenvalues and eigenvectors, respectively. By solving Eq. (9), we can obtain $\boldsymbol{E}$ and $U_{nl}(r)$.

In Table 1, we list the calculated p state energy values of H_0 obtained by using the B-spline technique and compare them with the results obtained

from the other model potential and the quantum defect method. It can be observed that the differences $|\Delta E|$ between our calculated energies and the other results are very small ($< 10^{-6}$ Hartree), which shows that our calculated results are very accurate. In Table 2, we list the principal numbers selected and the calculated Rydberg sodium atom levels of $n = 75, \ldots, 79$ states under the zero field.

Table 1. Calculated Rydberg sodium atom energy levels of p states under zero field (in Hartree).

n(p)	$E_{\rm MP}$	$E_{\rm MP1}$[20]	$E_{\rm QD}$[20]	$\lvert E_{\rm MP}-E_{\rm MP1}\rvert$	$\lvert E_{\rm MP}-E_{\rm QD}\rvert$
10	–0.005985186	–0.005985918	–0.005980573	7.32×10^{-7}	4.613×10^{-6}
11	–0.004862678	–0.004863214	–0.004859246	5.36×10^{-7}	3.432×10^{-6}
12	–0.004028748	–0.004029153	–0.004026129	4.05×10^{-7}	2.619×10^{-6}
13	–0.003392320	–0.003392633	–0.003390278	3.13×10^{-7}	2.042×10^{-6}
14	–0.002895608	–0.002895855	–0.002893987	2.47×10^{-7}	1.621×10^{-6}
15	–0.002500517	–0.002500715	–0.002499209	1.98×10^{-7}	1.308×10^{-6}
16	–0.002181103	–0.002181264	–0.002180032	1.61×10^{-7}	1.071×10^{-6}
17	–0.001919202	–0.001919335	–0.001918315	1.33×10^{-7}	8.87×10^{-7}
18	–0.001701792	–0.001701903	–0.001701049	1.11×10^{-7}	7.43×10^{-7}
19	–0.001519337	–0.001519431	–0.001518709	9.4×10^{-8}	6.28×10^{-7}
20	–0.001364727	–0.001364806	–0.001364191	7.9×10^{-8}	5.36×10^{-7}

Table 2. Calculated Rydberg sodium atom energy levels of $l = 1$ and $n = 75, \ldots, 79$ states under zero field (in Hartree).

n	$E_{\rm MP}$
75	–0.0000909602235
76	–0.0000885552825
77	–0.0000862444738
78	–0.0000840229482
79	–0.0000818861648

2.3. Solution of the time-dependent Schrödinger equation

By choosing eigenstates of H_0 as the new basis set, the time-dependent wavefunction of the sodium atom in the presence of microwave field can be written as

$$\psi(\boldsymbol{r}, t) = \sum_{k=1}^{n} a_k(t)\psi_k \, \mathrm{e}^{-\mathrm{i}E_k t}, \tag{10}$$

where $a_k(t)$ is the coefficient of the expansion, and it represents the amplitude of the transition probability. Then by substituting Eq. (10) into Eq. (1), we can obtain expansion coefficient $a_k(t)$ by solving the time-dependent Schrödinger equation numerically. The probability of the outer electron occupying state k at time t can be written as

$$P_k = |a_k|^2. \tag{11}$$

Using the above formula, we can obtain the state-to-state transition probability, from which we can observe the famous Rabi oscillation and some other interesting features directly.

3. Results

In this section, the population transfers of a sodium atom from a lower state ($n = 75$) to a higher state ($n = 79$) in chirped microwave fields are discussed. Firstly we investigate the population transfer of sodium atom in a microwave field with $m = 6$, $E_0 = 140$ V/cm, $\omega_0 = 17.8$ GHz, $\beta = -0.00095$ GHz/ns, and $T = 1.0\times10^{-5}$ ns. The obtained population transfer between the atom states is illustrated in Fig. 1(a), showing that about 99.88% of the $n = 75$ state atoms are transferred to the $n = 79$ state. In this process, five sequential adiabatic passages are formed by a single frequency-swept laser. The $n = 75$ state population is transferred to $n = 76$, 77, 78 states and finally comes to the $n = 79$ state. Next, changing to $\beta = -0.00085$ GHz/ns and keeping the other parameters unchanged, we find that about 97.07% of the $n = 75$ state atoms are transferred to the $n = 79$ state, as shown in Fig. 1(b). We can see that the population in the $n = 79$ state slightly oscillates with time and finally is stable there, which can be regarded as a small Rabi oscillation induced in the $n = 79$ state. From Figs. 1(a) and 1(b), we know that the population transition probability from the initial state to the final

state is related to the chirped rate β. Hence, to coherently control the population transfer, the chirped rate must be optimized. Then we change the number of the microwave pulse period into 5, i.e., $m = 5$, the other parameters are kept the same as those in Fig. 1(a), the obtained population is illustrated in Fig. 1(c). About 39.46% of the $n = 75$ state atoms are transferred to the $n = 79$ state. This shows that the population transition probability is related to the number of the microwave pulse period m. Figure 1(d), where $\omega_0 = 17.25$ GHz and the other parameters are kept the same as those in Fig. 1(a), shows that about 71.51% of the population is transferred to the $n = 79$ state. At the beginning of the process, a bigger oscillation arises between $n = 75$ and $n = 76$ states, which can be seen as a stronger Rabi oscillation. From all the figures, we know that the population transition probability from the initial state to the final state is related to chirped rate β, number of the microwave pulse period m, and initial frequency ω_0.

From the above analysis, we can draw the conclusion that the populations transferred to the final state are different for different parameters. An efficient population transfer can be realized and eventually trapped in the final state by modulating chirped rate β, number of the microwave pulse period m, and initial frequency ω_0, which shows that the coherent control of the population transfer from the lower states to the higher ones can be accomplished by optimizing the microwave pulse parameters.

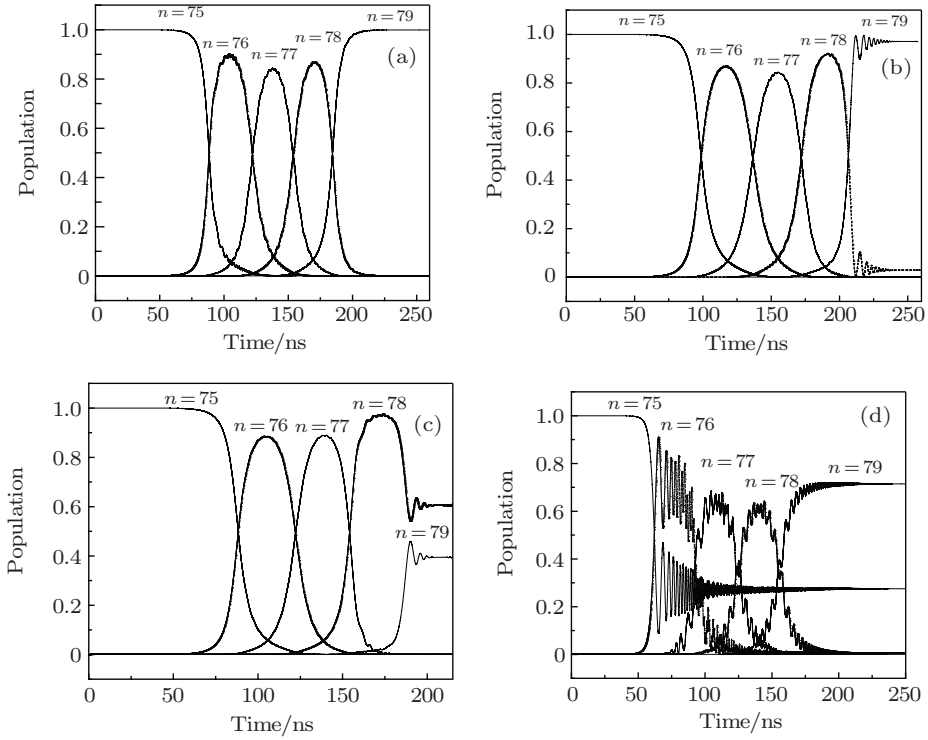

Fig. 1. Population transfers from $n = 75$ to $n = 79$ in a microwave field of frequency sweep. The parameters in panel (a) are $\omega_0 = 17.8$ GHz, $m = 6$, $E_0 = 140$ V/cm, $T = 1.0 \times 10^{-5}$ ns, and $\beta = -0.00095$ GHz/ns. In panel (b), β is changed to -0.00085 GHz/ns, in panel (c), m is changed to 5, and in panel (d), ω_0 is changed to 17.25 GHz.

4. Conclusion

In this paper, we calculate Rydberg sodium atom energy levels of p states in zero field by using the B-splines; the calculated results accord well with the other theoretical results. We demonstrate that the population can be transferred to a higher state efficiently by exposing the Rydberg sodium atoms to specially designed microwave pulses. We can draw the conclusion that the parameters of a microwave pulse have an important effect on the population transfer from the initial state to the final state. The coherent control of the population transfer from a lower n state to a higher n state can be accomplished by optimizing parameters β, m, and ω_0. So, it is possible to achieve the coherent control of the population transfer of the Rydberg sodium atoms by designing appropriate mi-

crowave pulses.

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