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Tunneling between double wells of atom in crossed electromagnetic fields*

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The tunneling between double wells of atom in crossed electromagnetic fields is investigated by a one-dimensional Hamiltonian model. The crossed fields induced outer well is apart from the nuclear origin and it is very difficult to access by means of spectroscopy but it will be possible if there exists the tunneling of the electron between the outer well and the Coulomb potential predominated well at the nuclear origin. A one-dimensional quantum calculation with B-spline basis has been performed for hydrogen atom in crossed fields accessible in our laboratory, at $B = 0.8$ T and $F = -220$ V·cm^{-1}. The calculation shows that the wavefunctions of some excited states close to the Stark saddle point in the outer well extend over to the Coulomb potential well, making it possible to penetrate the quantum information of the outer well. However, the tunneling rate is very small and the spectral measurement of the transitions from the ground state should be of a high resolution and high sensitivity.

Keywords: double well, tunneling, crossed fields

PACC: 3150, 3345B

1. Introduction

The quantum mechanics with double-well potentials is very interesting as it is closely related to the quantum character of tunneling between wells. This double-well system immersed in environment has many inimitable properties and has been extensively studied.[1−9] With the development of the technology to handle Bose–Einstein condensate (BEC) or semiconductor, more and more double quantum well systems can be created in micro- or mesoscopic scale.

Instead of to encage atom or molecule in a micro- or mesoscopic trap, double well can also be formed in a single atom artificially but the manipulatable object is replaced by electron in it. The rydberg atom in specially configured crossed electric and magnetic fields is a typical example for this case. Near the nuclear origin, the Coulomb potential predominates although it is distorted by the magnetic field. This potential well, for convenience, is referred to as the magnetically distorted Coulomb well (MDCW) while the additional well induced by the external crossed fields is away from the origin and referred to as the outer well.[10,11] This special double-well feature is adopted to provide a unique way for stabilizing simple matter-antimatter systems as the lifetime goes up to the order of one year.[10] A two-step switching on of an external electric field is also proposed to prepare a hydrogen atom in a superposition of states in outer well efficiently.[12] If one puts the simplest hydrogen atom in the crossed fields at the values that form double wells, one could measure some special and significant quantities, such as the zero point energy.

However, for the double-well state of the Rydberg atom, the average nuclear–electron separation is so large that the transition moments between the ground state in the Coulomb potential and the excited states in outer well are extremely small, making it very difficult to penetrate the outer well by direct spectroscopy.

As yet, no evidence is related to double well directly although many efforts have been made to investigate the large electric dipole moment states. The highly excited Rybderg atoms in crossed fields have large electric dipole moments and can be deflected by an inhomogeneous electric field,[13] but these states are beyond the Stark saddle point.[14] For the case of double wells of atoms in crossed fields, Fauth, Walther

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and Werner[15] chose to excite the atom to Rydberg states slightly below the Stark saddle point and the excited electron will tunnel to the outer well, forming large dipole moments. The first study with the hydrogen atom in strong crossed magnetic and electric fields shows that long-living states can reach well above the Stark saddle energy but without any sign of the saddle point nor a noticeable signature or effect of a long-range potential well.[16] Sharp-line spectra are also observed showing the existence of long-living final states high in the field-ionization continuum. Afterwards, the spectrum of double well has been recorded at $B = 0.4$ T and $F = -90$ V·cm^{-1} in the investigation of the ionization threshold[17] and at $B = 0.7$ T and F around 200 V·cm^{-1} in the research of quasi-Landau resonances[18] of rubidium Rydberg atoms in crossed electric and magnetic fields. No valuable signature is related to double well. We also made an attempt with barium in crossed fields.[19] We argue that below the Stark saddle point all transitions occur in MDCW and the detected ionization signal is also from the excited states in MDCW except at the energy near the saddle point where the ionization might occur in outer well because the electron can tunnel through the low barrier between wells, but such signal should be of low intensity. Therefore, experiments of high resolution and high sensitivity are preferred for this purpose, as well as careful analysis, as we will discuss later.

In this paper, we take a one-dimensional model to study the hydrogen atom in crossed electric and magnetic fields and to see whether it is possible to probe the outer well by tunneling between the Coulomb well and the outer well. As is well known, nearly all optical transitions take place only in the Coulomb well because the ground state is confined close to the nuclear while the upper excited state in outer well is separated from the MDCW by a thick barrier. Thus the outer well is transparent for the observer. There is an exception, however, if the wavefunction of the upper state in outer well extends through barrier to the MDCW by tunneling near the Stark saddle point.[10] If so, can we catch some things fleeing away from outer well and then some certain quantities might be measurable. Principally, this technique is applicable for all energy levels in outer well as the shape of the double well for Rydberg atoms in crossed fields is controllable by varying the electric and magnetic fields strength and every energy level can be tuned up to the saddle point.

2. Quantum model and calculation

The Hamiltonian of a hydrogen atom in crossing electric and magnetic fields $\boldsymbol{F}\times\boldsymbol{B}$ with $\boldsymbol{F}$ along x axis and $\boldsymbol{B}$ along z axis, in cylindrical coordinates, is

$$H = \frac{1}{2}\nabla^2 + \frac{1}{2}\gamma l_z - \frac{1}{\sqrt{\rho^2+z^2}} + fx + \frac{1}{8}\gamma^2\rho^2, \quad (1)$$

where γ is the magnetic field in atomic units, defined as $\gamma = B/c = B/2.35\times10^5$ with B in Tesla and f the electric field in atomic units, defined as $f = F/F_0 = F/5.14\times10^9$ with F in V·cm^{-1}. It can be seen that the linear Stark term fx and the quadratic Zeeman term are parabolic and can form a potential well at positive x position if appropriate values of fields taken. This outer well distinguishes from the well at nuclear origin of zero x position where the Coulomb potential predominates. As our interest perches on the tunneling between the two wells, the other two dimensions of y and z in Hamiltonian are omitted incipiently, namely, only the behaviour in the crossed line between planes $y = z = 0$ is considered. For simplicity, the paramagnetic term $\frac{1}{2}\gamma l_z$ is also removed if we assume $l_z = 0$. In this case, the Hamiltonian degenerates into

$$H = \frac{1}{2}\nabla_x^2 - \frac{1}{|x|} + fx + \frac{1}{8}\gamma^2x^2. \quad (2)$$

Figure 1 is the typical double well potential energy surfaces of hydrogen at different combined values of crossed electric and magnetic fields that can be achieved in our laboratory. It can be seen that the external fields induced outer well only exists at some certain values of crossed fields. As the energy is extremely sensitive to the fields applied, both of the magnetic field and the electric field should be stable enough for an experimental observation. Moreover, the spectral gaps of eigen-energies are also dependent on the strength of the fields, requiring a laser of corresponding resolution. For our laboratory, the lowest magnetic field strength for resolvable observation should run over 0.8 T and the electric field should rise up to -200 V·cm^{-1} as depicted in Fig.1.

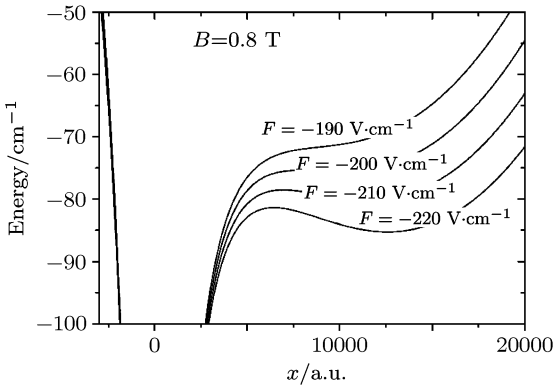


Fig.1. Typical potential energy surfaces of hydrogen in crossed fields that can be achieved in our laboratory. At $B = 0.8$ T, the double well is not present until the electric field strength increases up to $F = -200$ V·cm^{-1}. As the double well potential changes sensitively with the fields applied, an appropriate set of field values should be chosen according to energy gaps and laser resolution, for example, $B = 0.8$ T and $F = -220$ V·cm^{-1}, in our case.

To solve the Schrödinger equation $H\phi_f = E\phi_f$, we use the B-spline basis and complex rotation techniques, which have been well described in numerous references.[20−25] In contrast to Gaussian-type orbital (GTO) or Slater-type orbital (STO), which extends to infinity, B-spline basis is compact L^2 integrable functions defined in a finite space. The matrices in B-spline basis are usually sparse and have a banded structure. This feature avoids linear dependencies in the digitalization procedure and greatly reduces computation memories for matrix. Once the eigenwavefunction ϕ_f is determined, we can calculate the probability of the transition ρ from the ground state ϕ_i, $\rho = |\langle\phi_i| D |\phi_f\rangle|^2$. To approach the ground state of the real atom, barium, used in our experiment, the 6s state wavefunction of hydrogen is taken, especially to characterize the space size of the electron cloud.

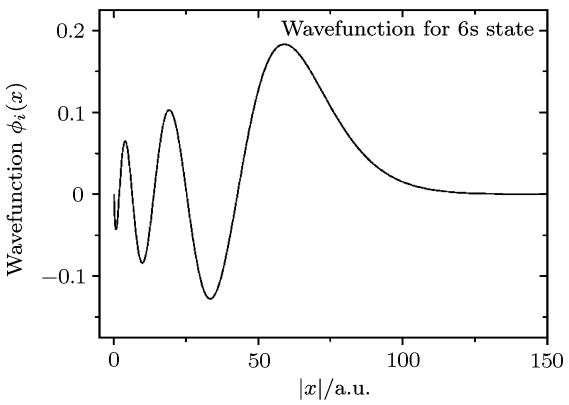


Fig.2. The wavefunction of the ground state used in our model. It is taken to be as 6s state of hydrogen to well characterize the volume size of the ground state of barium used in our laboratory.

It is displayed in Fig.2. It can be seen that the wavefunction is squashed in a small volume of less than 120 a.u., implying that the wavefunction of the upper states for the effective transition from the ground state should at least have a considerable distribution in this area.

3. Results and discussion

The calculated transition spectrum is shown in Fig.3 and the corresponding energy level diagram shown in Fig.4. In the calculation, a Doppler broadening of 0.03 cm^{-1} is inserted according to the laser linewidth and the gating width of the time of flight detection for the excited atoms. The parameters for the double well potential are taken as $B = 0.8$ T and $F = -220$ V·cm^{-1}. We can notice from Fig.3 that dense lines come out to being when energy $E > -81.5$ cm^{-1}. The critical change across this energy is magnified in the sub-window of Fig.3. With the help of the energy levels shown in Fig.4, one can see that the critical energy is close to the classical Stark saddle point formed by crossed electric and magnetic fields. The calculation gives a spectral line at energy $E = -81.709$ cm^{-1}, but it is very weak, even un-observable in the calculated spectrum shown in Fig.3. However, this line gives a wavefunction that can connect MDCW and outer

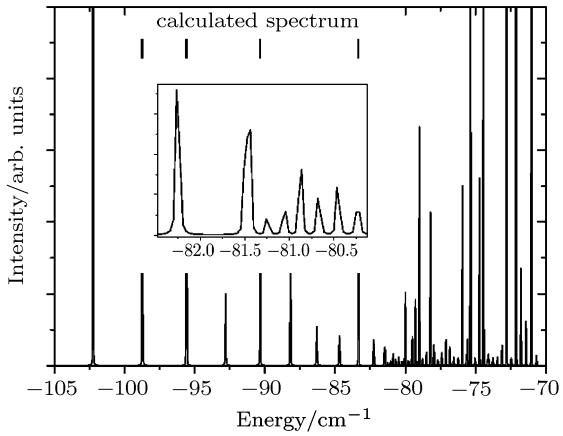


Fig.3. The spectrum calculated with one-dimensional model. The transitions are from the ground state 6s to the upper excited states. It can be seen that the spectral lines gets dense after crossing over the critical energy $E = -81.5$ cm^{-1}, which is magnified in the inset.

well in space but with the same eigenenergy. It corresponds to the eigen-energy of $v = 12$ in outer well. Its wavefunction is depicted in Fig.5(a), where one

can see that the wavefunction has much larger oscillation amplitude in outer well than in MDCW and the contribution in MDCW for the transition is not strong enough to give an observable spectral line. For the spectral lines at energy $E = -81.4972$ cm^{-1} and $E = -81.4454$ cm^{-1}, however, the wavefunctions extend over to both wells, even the barrier area at the saddle point, which are shown in Figs.5(b) and 5(c). In these cases, they can give considerable spectral intensities. They correspond to the same eigen-energy of $v = 13$ in outer well.

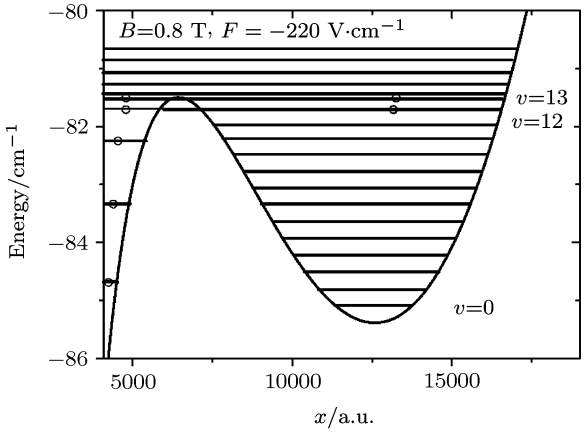


Fig.4. The energy level diagram across the Stark saddle point. The outer well is separated from the MDCW and cannot be accessed by optical transition from the ground state in MDCW; but near the saddle point, it gets possible through the tunneling between outer well and MDCW.

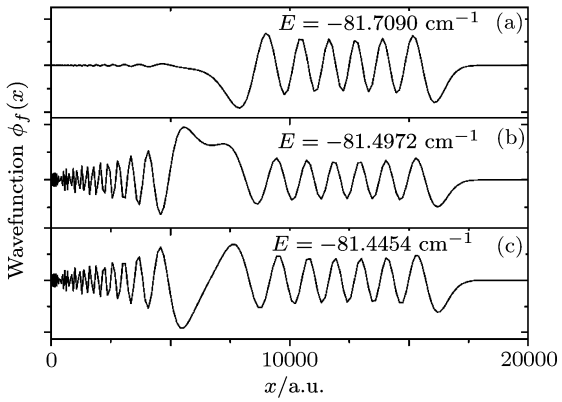


Fig.5. The wavefunctions of the excited states close to the Stark saddle point at various eigen-energies. Figure 5(a) shows the wavefunction prevailing in outer well, the transition probability being too small to be observable in the spectrum as shown in Fig.3. Figures 5(b) and 5(c) display the wavefunctions which extend over the whole range, even within the barrier area. They are observable.

As is well known, any measurement is actualized through interaction between that to be investigated and the observer. Now, in our case, the available transition used for observation occurs in MDCW, but if the wavefunction of outer well has a weak leaking through the barrier, we can peer the information of outer well indirectly. This is well understood in many spectroscopic observations, for example, the avoided crossing spectrum of CS^+ observed by us previously,[26,27] where the wavefunction is shared by additional energy level. Therefore, we can observe another spectral line due to wavefunction mixing. Another example is the electric-field-induced avoided level crossings in helium Rydberg states, where the spectrum is divided into two manifolds and the neonatal one absorbs most of the oscillator strength at the cost of Stark states in the middle of the manifold.[28] This avoided crossing is also observed in diamagnetic hydrogen.[29] This kind of potential-curve-crossing problem has been extensively discussed by Delos.[30] The only difference from our case is that the transition to the outer well is forbidden, so the shared wavefunction only contribute to the transition occurring in the MDCW and one cannot observe the spectral line due to wavefunction staying in outer well. This is, on the contrary, the case to provide a unique way for stabilizing simple matter-antimatter systems,[10,11] where the wavefunction leaking from the outer well should be prohibited to prolong the lifetime of the double well system of matter-antimatter.

Like the usual spectral observation for avoided crossing levels, the pick-up for this kind of lines from the experimental observation relies on the well-understanding for the spectrum in the whole energy range.[26,27] Therefore, an unambiguous assignment for the experimental spectrum should be done at energies away from the interaction at the Stark saddle point. From this point, a well theoretical understanding for the atoms interested is required and a high dimensional calculation for spectrum is preferred by diagonalization of large matrices[31] or by time-dependent approach.[32]

However, there should be some differences between the spectrum calculated by one-dimensional model and that of one real atomic system. In a one-dimensional model, there is only one channel to cross the barrier at the saddle point, while there might be more complicated movement of electron in high dimensions; for example, in 2-dimensions, where only the movement in pure Coulomb potential in z direction is omitted. The tunneling in x direction may be achieved through back and forth in y direction, where

the potential is distorted by magnetic field. Analytically, the wavefunction of the real atomic system can be written as the product of the wavefunctions in the x-, y- and z-directions. In the area of small r, corresponding to the MDCW energy levels lower than the tunneling, according to the Hamiltonian given in Eq.(1), as the Coulomb potential predominates, the one-dimensional calculation should be close to the real atomic system. On the contrary, in the area of large r, corresponding to the outer well energy levels, the outer well in the x-direction comes to play the role. For the energy levels lower than the saddle point in outer well along the x-direction, they are correlated with the other two-directions through the Coulomb potential term and the spectral intensity should be scaled by the product of the wavefunction in the y- and z-directions. Consequently, the one-dimensional calculation cannot give reliable spectral intensity information, if it is compared with an experimental observation. For the energy levels above the saddle point, the outer well can be approximately separated from the other directions as the Coulomb potential is small, comparatively. So the energy gaps between spectral lines should be close to that of the real system. This analysis suggests that the spectral lines of the real atomic system might not be exposed regularly as the inset shown in Fig.3, but the spectral line position could make sense for the experimental observation.

Recently, we have made an experimental investigation on quasi-bound electrons in crossed electric and magnetic fields, in which states of very large electric dipole moment are excited.[19] Although the laser has a narrow linewidth of 400 MHz, we have to use a low magnetic field of 0.3 T because the static magnetic field is produced by a solenoid electromagnetic magnet with wicked stability. It results in that it is very difficult to hunt the fine structure from the scanned spectrum.

Additionally, as the second well is very wide and the eigenenergy gap is very small under usually available experimental conditions, the measurement should be of high resolution. This can be estimated by the formula given in Ref.[33]. In the case of double well, the electron of atom in outer well is far away from the nuclear origin and the energy shift induced by the crossed fields is given by $\delta E = -2F^2/B^2$. A rough estimate shows that the harmonic oscillator energy gap due to diamagnetic term in Eq.(1) is about 0.14 cm^{-1} at $B = 0.3$ T and a high resolution laser should be used. Furthermore, under the double well condition, namely, at $F = -125$ $\mathrm{V{\cdot}cm}^{-1}$, the required stability is around 0.05 $\mathrm{V{\cdot}cm}^{-1}$ for electric field and 2.5×10^{-6} T for magnetic field. This is why we could not obtain any fine structure at low magnetic field.[19] However, if we take the parameters of $B = 0.8$ T and $F = -220$ $\mathrm{V{\cdot}cm}^{-1}$ for double well, the demand for the stability of magnet begins to reduce and it will be 2.7×10^{-5} T, which can be achieved by a superconducting magnet. However, higher magnetic field will ask for higher electric field to form double well, which will be very difficult to keep constant in experiment. So it is vital to choose appropriate values of crossed fields if an experimental approach is programmed.

4. Conclusion

We have investigated the tunneling between double wells of atom in crossed electromagnetic fields by a one-dimensional Hamiltonian. As usually proposed, the tunneling between the two wells supplies a method to link up with the outer well of atom in crossed electric and magnetic fields, giving a chance to get at it by observable spectral transitions in MDCW. The quantum calculation of spectrum on hydrogen atom at available condition $B = 0.8$ T and $F = -220$ $\mathrm{V{\cdot}cm}^{-1}$ shows the wavefunction in the outer well will extend over to the MDCW at the Stark saddle point, but the tunneling rate is very small and the spectral observation should be an experimental challenge. However, this calculation gives an understanding for the spectrum theoretically, which helps discriminate the tunneling signal from the observed spectrum if it is experimentally possible. On the one hand, the potential energy surface is sensitive to the applied electric and magnetic fields, one has to choose a higher magnetic field to achieve a large harmonic oscillator strength. On the other hand, a higher magnetic field for a double well potential requires a higher electric field, at which value it is not easy to keep constant with high stability. Therefore, appropriate values of both electric and magnetic fields should be determined for a feasible experiment, e.g., $B = 0.8$ T and $F = -220$ $\mathrm{V{\cdot}cm}^{-1}$ for our case.

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