## **Physics 860** Take-home Final Examination

1:30-6:30pm, Wed. May 11, 2005

(Each question worths 20 points, be precise and concise)

## Problem-1. Dissociation and Ionization of $H_2^+$

I will ask a few more questions on this system. Here are some of the figures that you have seen before. You will use

them to answer the questions below.



fig. 2

fig.3

Fig. 2 shows the kinetic energy spectra per proton from Gibson et al (1997). In the class we attributed the broad peak on this figure centered at 2.0 eV to be due to the CREI. The result from Fig.3 shows that CREI peaks at internuclear distance of about 6-10 a.u. We will take it to be at 8 a.u.

(a) If the  $H_2^+$  is ionized directly from R=8 a.u., what is the kinetic energy per proton? You will find it is not 2 eV/proton.

(b) According to Frank-Condon principle, it is not easy for the  $H_2^+$  to reach 8 a.u. directly. Why is so?

(c) One way to reach 8 a.u. is a two-step process. As the  $H_2^+$  moves to a distance where the 1s  $\sigma$  and 2p  $\sigma$  potential curves are separated by the energy of one photon, the  $H_2^+$  can be populated to the 2p  $\sigma$  curve. For the 790 nm laser, using Fig.1, at what distance in R does this occur?

(d) Now  $H_2^+$  will follow the 2p  $\sigma$  curve to R=8 a.u.. From Fig.1 read what is the kinetic energy as it reaches that distance? Express your answer in eV.

(e) Add the kinetic energy from part (d) to what you get on part (b), and show that you can recover the energy of about 2 eV/proton for the CREI as in Fig. 2.

(f) Explain why this CREI peak is so broad.

(g) If the laser polarization is perpendicular to the molecular axis, do you expect to see the spectra as shown in Fig.2? (Hint: you need to recall the selection rule for transition between two molecular curves -- very simple one.) Be specific, and explain the reason.

(h) If the  $H_2^+$  ions were prepared initially at the v=2 state, what would be the expected spectra if the kinetic energy of the proton is measured?

(i) If the laser wavelength is halved, answer part (h) again. Give your reasons.

(j) If the laser wavelength is halved to 395 nm, from Fig.1 estimate what would the low-energy dissociation peaks look like? Assume that the initial distribution of the vibrational states is Frank-Condon. Which v will be seen first (For 780nm, it was v=5)?

(k) For 395nm pulse, would the CREI peak appear at the same energy region or would it shift to a different value? What value? (Recall how you did part (c) and (d)). [bonus question: worth's 10 points]

## Problem-2. Ionization in two-color XUV+IR fields

We use a 0.1fs XUV pulse to ionize an atom to create an inner-shell hole. This inner-shell atom will eject an Auger electron. Without the presence of the IR laser, the Auger electron will have an energy of 50 eV. Assume that the peak electric field of the IR laser is 0.05 a.u.

You want to do the time-resolved experiment. Assume that the laser is the 5fs, 800nm pulse and the XUV has 95 eV mean energy. You want to vary the time delay of the IR with respect to XUV over one optical cycle starting from the peak of the laser field.

Assume that the Auger lifetime is 0.15 fs and the electron is measured in the forward direction.

(a) What is the width of the Auger electron if no laser is present?

(b) What is the electron spectrum like when the XUV is at the peak of the laser's electric field?

(c) What is the electron spectrum like when the XUV is centered at the point where the laser's electric field is zero?

Repeat the answer to the three questions above if the lifetime of the Auger electron is 15 fs.

## Problem-3. Ionization of Ar by circularly polarized light

(a very easy one if you are not on the wrong track.)

For a left circularly polarized light with pulse duration of 5 fs, and carrier-envelope phase  $\phi = 0$ , write down the expression of the electric field **E**(t), assuming that it is a Gaussian pulse. Take the peak electric field to be 0.1 a.u. If you use such a pulse to ionize the Ar atom, what is the direction of the emitted electrons? Answer the same question if  $\phi = 90^{\circ}$ 

**Problem-4.** Use the simple computer programs from homework-5 to make these calculations. [This will take more time to do-- so do it at the end.]

(a) Calculate the alignment-dependent ionization rates for  $O_2$  molecules at peak intensity of  $2x10^{14}$  W/cm<sup>2</sup>. Show the graph.

(b) What is the saturation intensity of  $O_2$  when it is aligned by  $45^\circ$  with respect to the laser polarization direction? Assume that the pulse length is 45 fs.

**Problem-5. Molecular clock by the rescattering process**. Refer to homework-7. Read the left column first and then answer the questions on the 2nd column.



This figure was taken from the experiment of Corkum's group, Nature 2003. What is shown is the kinetic energy release <u>per deuteron</u> (they used  $D_2$  molecules). <u>Using the model in homework-7</u>, we want to deduce what is the average vibrational level of the initial  $D_2^+$  wave packet. We will assume that the second ionization is by the rescattering process, and the peak is due to the recattering occurring at the third return, or  $t_3$ .

(a) What is the internuclear distance at which the second ionization occurs for each wavelength?

(b) If we assume that the 2nd ionization occurs at time  $t_3$ , what is the time interval between the two ionizations for each wavelength?

Now consider the 1850nm case: (c) How much the internuclear distance has increased between the two ionizations?

(d) If you treat the vibrational wave packet as a classical harmonic oscillator, what is the amplitude of the oscillation of this oscillator?

(e) What is the total energy of this wave packet? What vibrational state does it correspond to?

(you can use the results from homework-7)