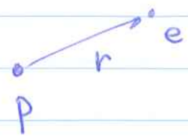
Hydrogen atom (brief reminder)




Coulumb interaction $U(r) = -\frac{ke^2}{r}$

Kinetic energy $K = \frac{p^2}{2\mu}$

$$\mu = \left(\frac{1}{m_e} + \frac{1}{m_p}\right)^{-1} \approx m_e\left(1 + \frac{m_e}{m_p}\right)$$

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{ke^2}{r}$$

Shrodinger equation $\hat{H}\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$

$$\hat{H}\psi = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2 r\psi}{\partial r^2} - \frac{1}{2\mu r^2}\hat{L}^2\psi - \frac{ke^2}{r}\psi = E\psi$$

As expected for the spherically symmetric potential, $\hat{H}$ commutes with $\hat{L}^2$ (and $\hat{L}_z$)

Thus, we can identify the eigenstates of this potential using three quantum numbers: $n, \ell, m_\ell$, such that

$$\hat{H}\psi_{n\ell m} = -\frac{E_R}{n^2}\psi_{n\ell m}$$

$$\hat{L}^2\psi_{n\ell m} = \hbar^2\ell(\ell+1)\psi_{n\ell m} \qquad \hat{L}_z\psi_{n\ell m} = \hbar m\psi_{n\ell m}$$

where $\ell = 0 \ldots n-1$, and $-\ell \le m \le \ell$ are integer numbers

$$\psi_{n\ell m} = R_{n\ell}(r)\,Y_{\ell m}(\theta,\varphi)$$

$Y_{\ell m}(\theta,\varphi)$ - orthonormal spherical functions

$$\int Y^*_{\ell m}(\theta,\varphi)\,Y_{\ell' m'}(\theta,\varphi)\,d\Omega = \delta_{\ell\ell'}\delta_{mm'}$$

~~Each~~

Each energy state $E_n = -\frac{E_R}{n^2}$ is $n^2$ time degenerate
(actually, $2n^2$, considering spin)

Also, each state has distinkt parity $\mathcal{P}\psi_{nlm} = (-1)^l \psi_{nlm}$

Possible corrections

a) H-atom interacts with an outside world
- magnetic field (Zeeman effect)
- electric field (Stark effect)
- neighbouring atoms (van-der-Waals interactions)

b) Relativistic corrections

- Correction to the kinetic energy
- Spin !
  Spin-orbit coupling (Fine structure)

  Hyperfine structure (electron-nuclea spin-orbit coupling)
- Correction due to finite nuclei size

c) QED corrections (Lamb shift, wait till grad school)

H-atom in magnetic field
( so far for a spinless electron )

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2\mu} - \frac{ke^2}{r}}_{\hat{H}^{(0)}} - \underbrace{\hat{\vec{\mu}}_L \vec{B}}_{\hat{H}'}$$

Magnetic moment $\vec{\mu} = -\frac{e}{2m_e c}\vec{L}$

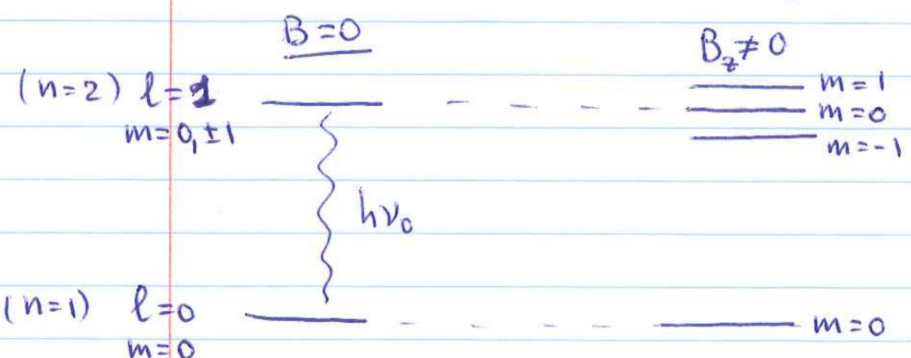
Choosing $\vec{B}$ in z-direction $-\hat{\vec{\mu}}_L \vec{B} = \frac{e}{2m_e c} B_z \hat{L}_z$

$$\hat{H}' = \frac{e}{2m_e c} B_z \hat{L}_z$$

→ $\psi_{\cancel{e}nlm}$ are eigenfunctions of $\hat{H}'$ already, so we only going to have the first-order correction

$$E^{(1)}_{nlm} = \langle \psi_{nlm} | \hat{H}' | \psi_{nlm} \rangle = \frac{eB_z}{2m_e c} \langle \psi_{nlm} | \hat{L}_z | \psi_{nlm} \rangle$$

$$E^{(1)}_{nlm} = \frac{eB_z}{2m_e c} \hbar m$$




Magnetic field lifts the degeneracy of ~~diffe~~ levels with different m.

If an electron transitions from an excited state to a ground state, for B=0 there will be only one frequency $h\nu_0 = \frac{E_R}{n_{ground}} - \frac{E_R}{n_{excited}}$

But for $B \neq 0$ there will be three lines

$h\nu_0$, $h\nu_0 \pm \frac{eB_z\hbar}{2m_e c}$

# Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States

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To describe the microscopic properties of matter, quantum mechanics uses wave functions, whose structure and time dependence is governed by the Schrödinger equation. In atoms the charge distributions described by the wave function are rarely observed. The hydrogen atom is unique, since it only has one electron and, in a dc electric field, the Stark Hamiltonian is exactly separable in terms of parabolic coordinates ($\eta$, $\xi$, $\varphi$). As a result, the microscopic wave function along the $\xi$ coordinate that exists in the vicinity of the atom, and the projection of the continuum wave function measured at a macroscopic distance, share the same nodal structure. In this Letter, we report photoionization microscopy experiments where this nodal structure is directly observed. The experiments provide a validation of theoretical predictions that have been made over the last three decades.

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The main results of the experiments are shown in Fig. 3. In this figure calculated and experimental results are shown for four experiments, where the hydrogen atoms were excited to the $(n_1, n_2, m) = (0, 29, 0)$, $(1, 28, 0)$, $(2, 27, 0)$ and $(3, 26, 0)$ quasibound Stark states. As indicated in Fig. 3, the states lie at energies of $-172.82\ \mathrm{cm}^{-1}$, $-169.67\ \mathrm{cm}^{-1}$, $-166.45\ \mathrm{cm}^{-1}$, and $-163.30\ \mathrm{cm}^{-1}$ with respect to the field-free ionization limit, i.e., just above the saddle point

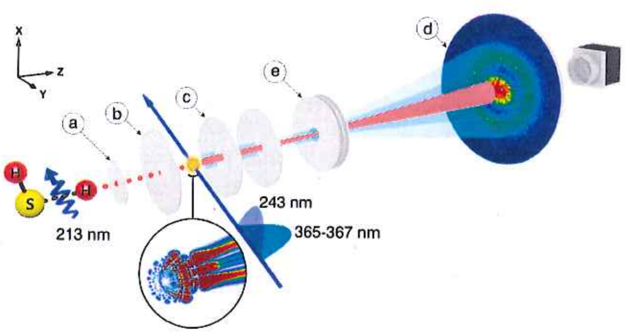


FIG. 2 (color online). Schematic overview of the experiment. An atomic hydrogen beam was formed by photodissociating $H_2S$ and placing a 3 mm aperture (a) 65 mm downstream. In the active region of a velocity map imaging (VMI) spectrometer, the ground state hydrogen atoms were first excited to a mixture of $n = 2$ $s$ and $p$ states by a two-photon transition using a pulsed 243 nm laser. Next, they were ionized by a Fourier-limited, tunable (365–367 nm), UV laser. By applying a voltage difference across the repeller (b) and extractor (c) electrodes, the photoelectrons were accelerated towards a two-dimensional detector (d), consisting of a set of microchannel plates (MCPs), a phosphor screen and a CCD camera. En route to the MCP detector, the photoelectrons passed through a three-element Einzel lens (e), allowing an increase of the diameter of the recorded image by about one order of magnitude.

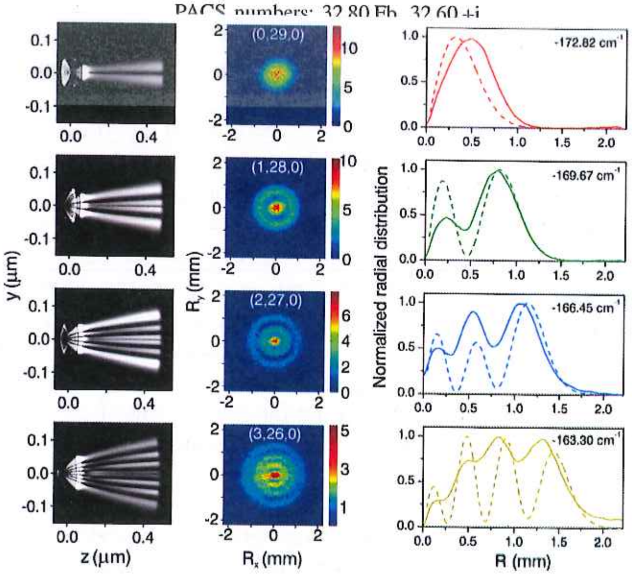


FIG. 3 (color online). Experimental observation of the transverse nodal structure of four atomic hydrogen Stark states. The images in the middle show experimental measurements for $(n_1, n_2, m) = (0, 29, 0)$, $(1, 28, 0)$, $(2, 27, 0)$, and $(3, 26, 0)$. Interference patterns are clearly observed where the number of nodes corresponds to the value of $n_1$. The results may be compared to TDSE calculations shown to the left (for details see text), revealing that the experimentally observed nodal structures originate from the transverse nodal structure of the initial state that is formed upon laser excitation. A comparison of the experimentally measured (solid lines) and calculated radial (dashed lines) probability distributions $P(R)$ is shown to the right of the experimental results. In order to make this comparison, the computational results were scaled to the macroscopic dimensions of the experiment. Please note that, since $P(R) = \int P(R, \alpha) R d\alpha$, the radial probability distributions $P(R)$ have a zero at $R = 0$, even if the two-dimensional images $P(R, \alpha)$ do not.