12.추가양자수

화공과 김영훈 교수

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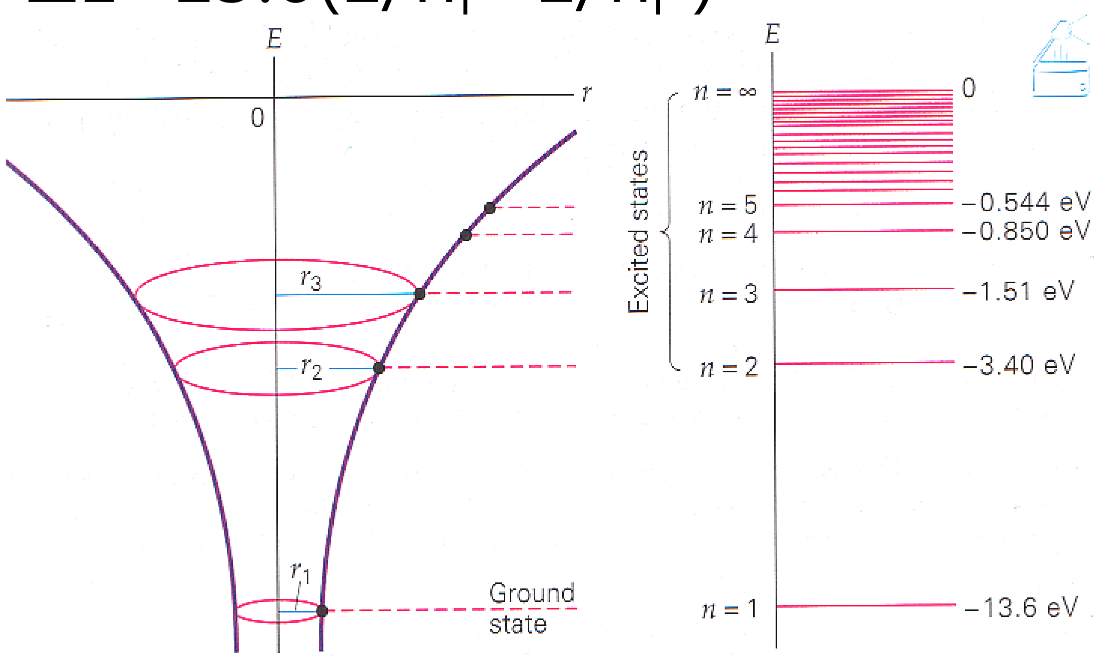
궤도(orbital) 개념

- $r_n = 0.0529n^2$ (nm)
- $E_n = -13.6/n^2$ (eV)
- Energy difference between the levels $\Delta E = 13.6(1/n_f^2 - 1/n_i^2)$



Initial State, n_i

ΔE=10.2 eV

Final state, n_f

타원방정식

- 타원(ellipse)
  - 평면위 초점에 이르는 거리의 합이 일정한 점의 자취
  - 장축길이 2a, 단축길이 2b, 초점 $c=(a^2-b^2)^{1/2}$

$$\overline{FP}+\overline{F'P}=2a(\text{단, } a>c>0)$$

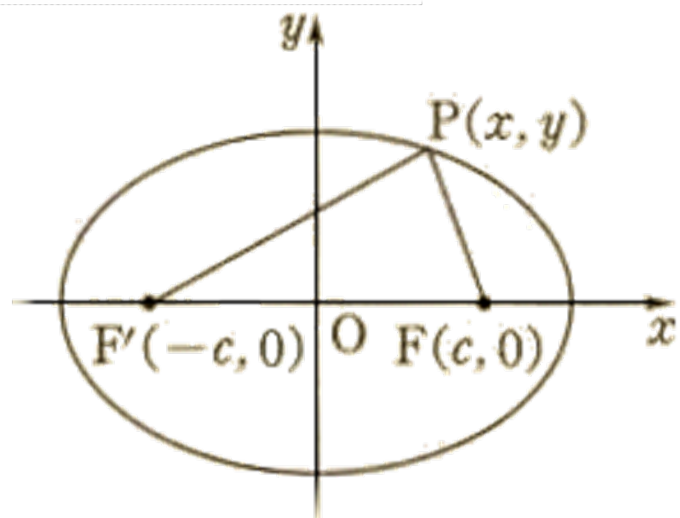
여기서, $\overline{FP}=\sqrt{(x-c)^2+y^2}$, $\overline{F'P}=\sqrt{(x+c)^2+y^2}$ 이므로,

$$\sqrt{(x-c)^2+y^2}+\sqrt{(x+c)^2+y^2}=2a$$

$$\sqrt{(x-c)^2+y^2}=2a-\sqrt{(x+c)^2+y^2}$$

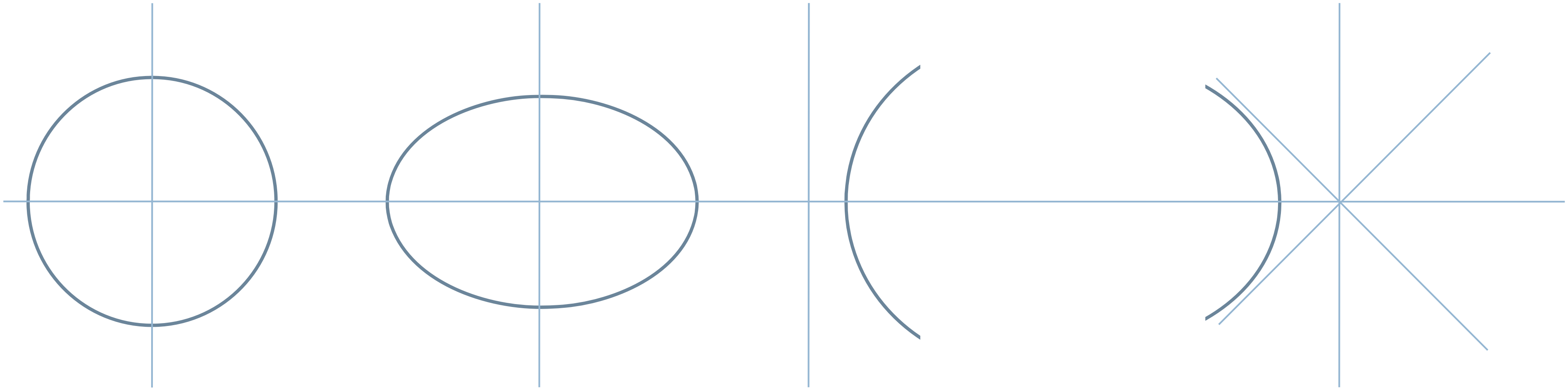
$$(a^2-c^2)x^2+a^2y^2=a^2(a^2-c^2)$$

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}=1(\text{단, } b^2=a^2-c^2)$$



회전체의 운동에너지

- E_k 커질수록 궤도 변경됨
  - 원 → 타원 → 포물선 → 쌍곡선



$$E = |E_k| = \frac{1}{2}|E_p| \qquad \frac{1}{2}|E_p| < E < |E_p| \qquad E = 0 \qquad E > |E_p|$$

수소 휘선의 미세구조(fine structure)

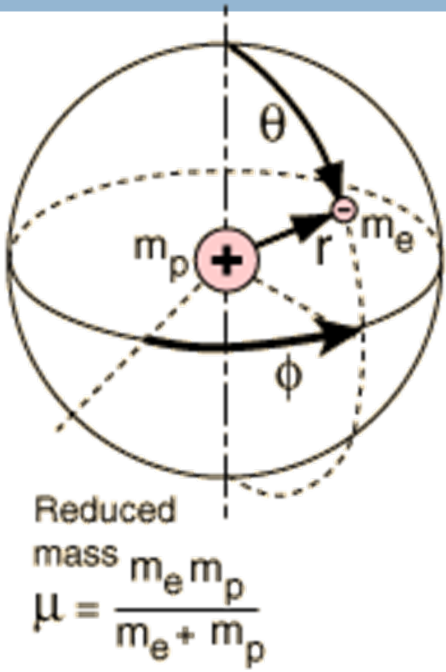
- 보어모델: 수소의 미세구조 설명 불가
- Bohr-Sommerfeld model
  - Single energy state는 사실 매우 근접한 여러 개의 energy state의 합이다
  - 원궤도에서 타원궤도로 수정
- 극좌표계(polar coordination): (r, θ)에 적용
  - $\oint L d\theta = n_\theta h \rightarrow L = \frac{h}{2\pi} n = n\hbar$
  - $\oint p_r dr = n_r h \rightarrow L(a/b - 1) = n\hbar$

Orbital quantum number, l

- From $\dfrac{mv^2}{r} = \dfrac{1}{4\pi\varepsilon_0}\dfrac{Ze^2}{r^2}$
  - 타원의 장축, 단축 좌표와 에너지 값

$$a = \frac{4\pi\varepsilon_0 n^2 \hbar^2}{\mu Z e^2},\ b = a\frac{n_\theta}{n},\ E = -\left(\frac{1}{4\pi\varepsilon_0}\right)^2 \frac{\mu Z^2 e^4}{2n^2\hbar^2}$$

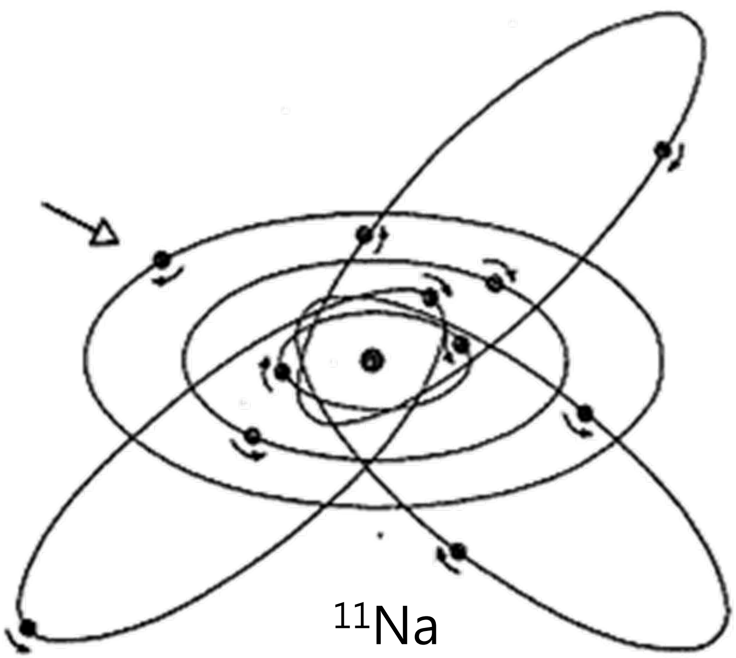
  - 오비탈의 모양은 n_θ/n 비로 결정



- 주양자수(principal quantum number) 성분
  - $n \equiv n_\theta + n_r$
  - $l = n_\theta - 1$: azimuthal quantum number (0,1,2,..,n-1)

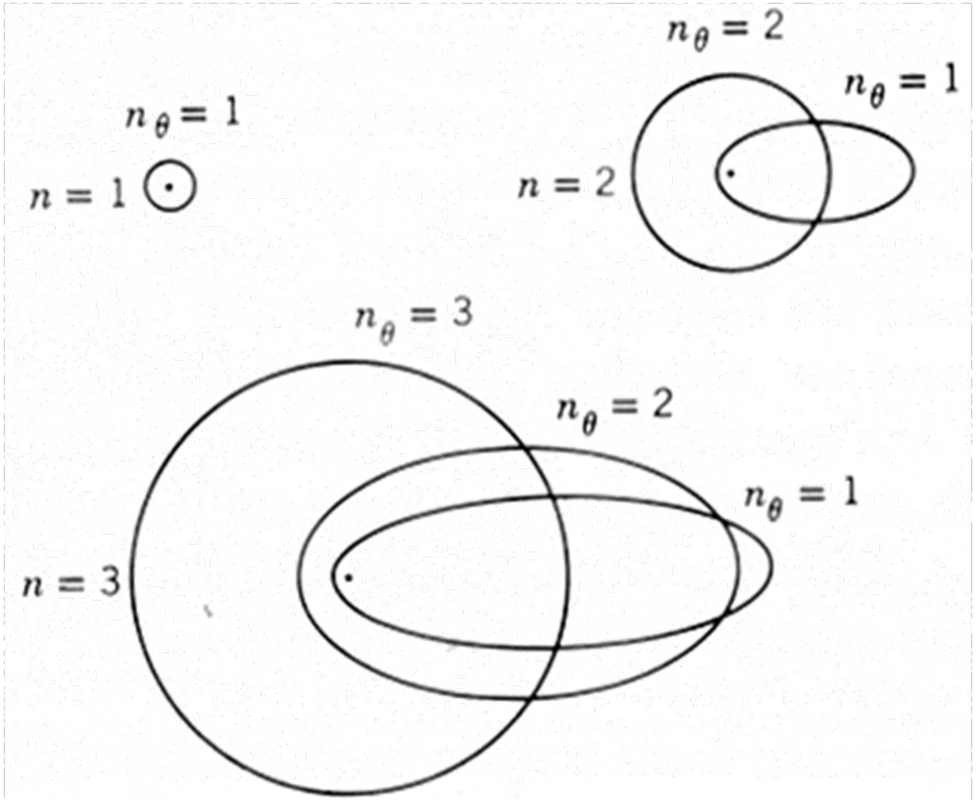
양자수 고려한 원자궤도

- Shape of orbit: n_θ/n ratio로 결정
  - $n_\theta=n$일때, 원형 궤도 → a=b
- 그러나, 궤도 모양에 무관하게 동일 주양주수 내 에너지 동일?



^{11}Na

$1s^2, 2s^2, 2p^6, 3s^1$



Degeneracy of orbit

- Way to removal of degeneracy
  - Relativistic correction: v/c~10^{-2}

$$E_n = -\frac{\mu Z^2 e^4}{2(4\pi\varepsilon_0)^2 \hbar^2}\frac{1}{n^2}\left[1+\frac{\alpha^2 Z^2}{n}\left(\frac{1}{n_\theta}-\frac{3}{4n}\right)\right]$$

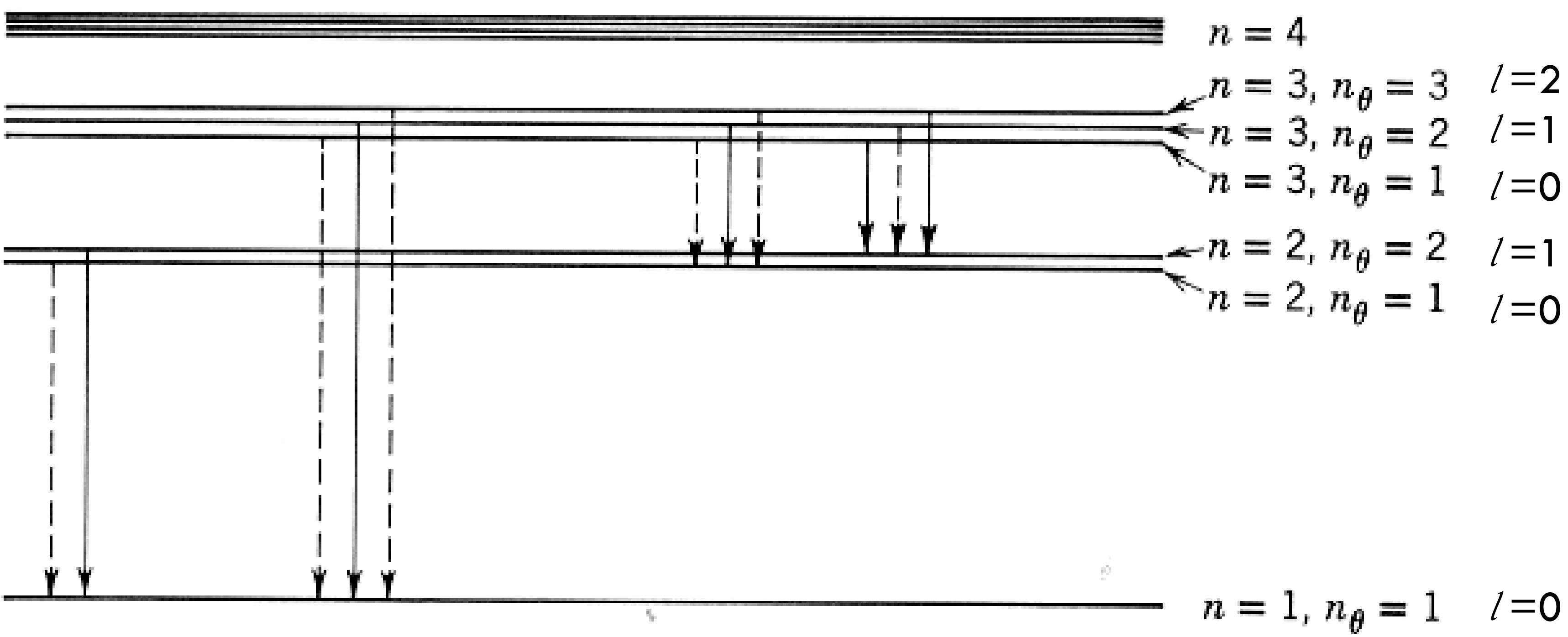
  - 식의 [ ] 부분이 궤도 모양 차이 보정항

  - Fine structure constant

$$\alpha \equiv \frac{e^2}{4\pi\varepsilon_0 \hbar c} = \frac{1}{137}$$

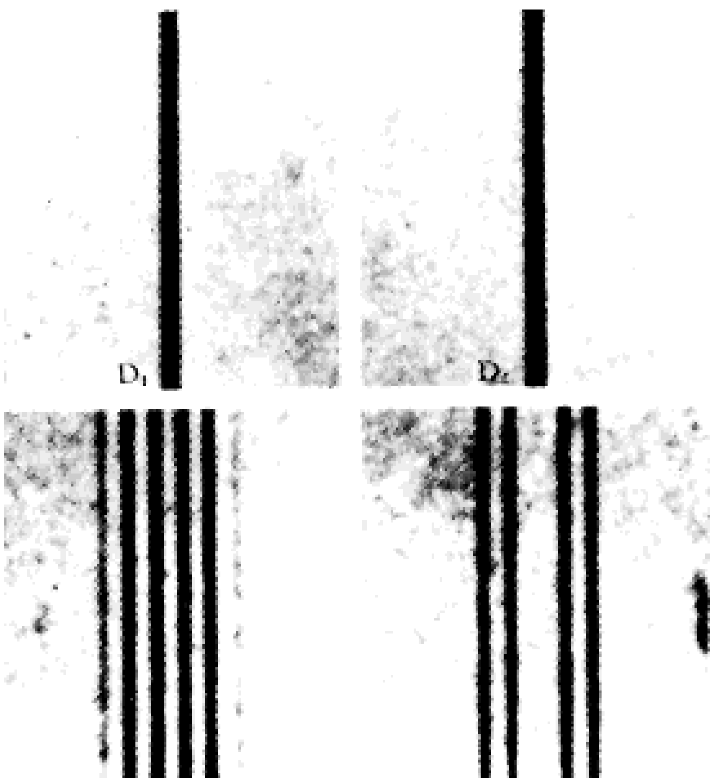
Selection rule

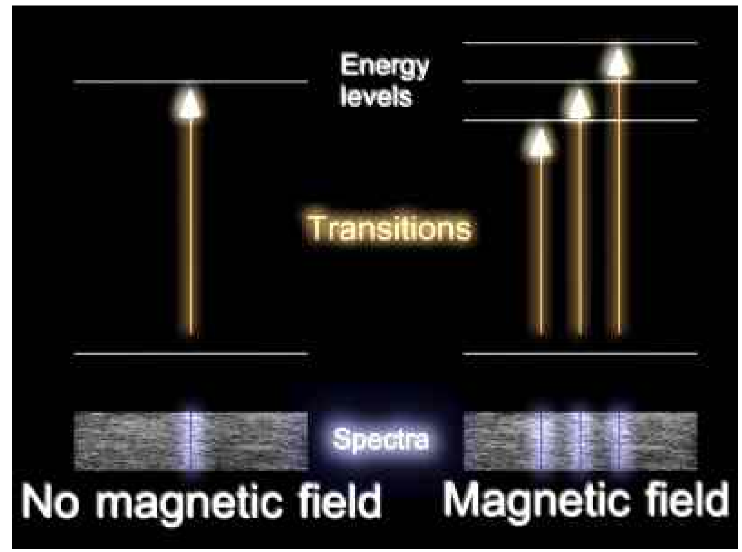
- 전자 전이: 전자기파 발생
  - 모든 전이를 관찰 가능한 것은 아니다
  - Selection rule이 지배, $n_{\theta i} - n_{\theta f} = \pm 1$

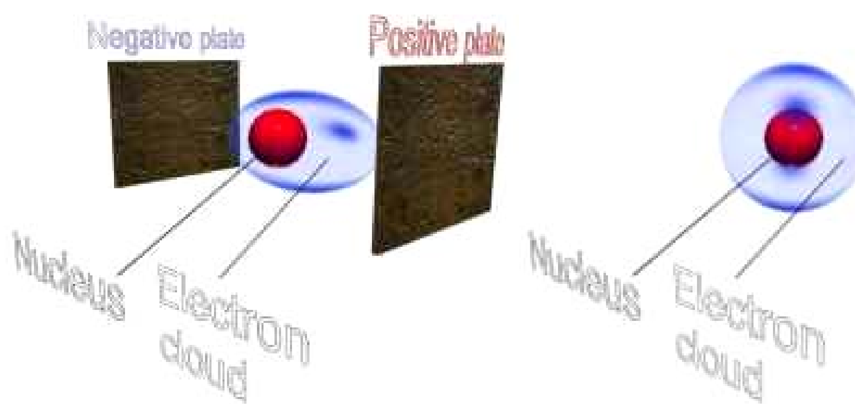


자기장에서의 스펙트럼 분리

- 자기장 하에서 더 많은 스펙트럼 선 관찰





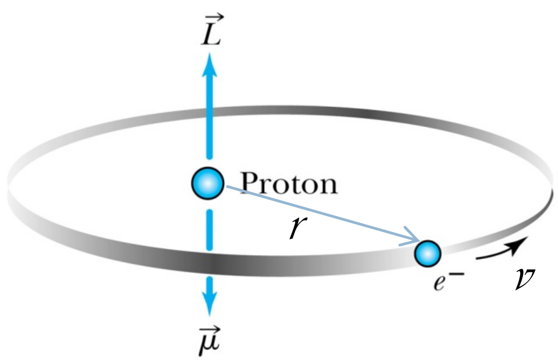


Magnetic potential energy

- Orbiting electron은 current loop 처럼 행동
  - Magnetic moment interaction energy 발생

$$I = \frac{qv}{2\pi r} = -\frac{ev}{2\pi r}$$

$$\mu = IA = -\frac{ev}{2\pi r}\pi r^2 = -\frac{e}{2m_e} m_e v r = -\frac{e}{2m_e} L$$



  - z 방향만 고려시

$$U(\theta) = -\mu \cdot B \qquad U = \frac{e}{2m} L_z B = m_\ell \frac{e\hbar}{2m} B$$

$$\Delta E = m_\ell \frac{e\hbar}{2m} B = m_\ell \mu_B B \qquad \mu_B = \text{Bohr magneton}$$

$$\mu_B = \frac{e\hbar}{2m_e} = 9.2740154 x 10^{-24} J/T = 5.788382 x 10^{-5} eV/T$$

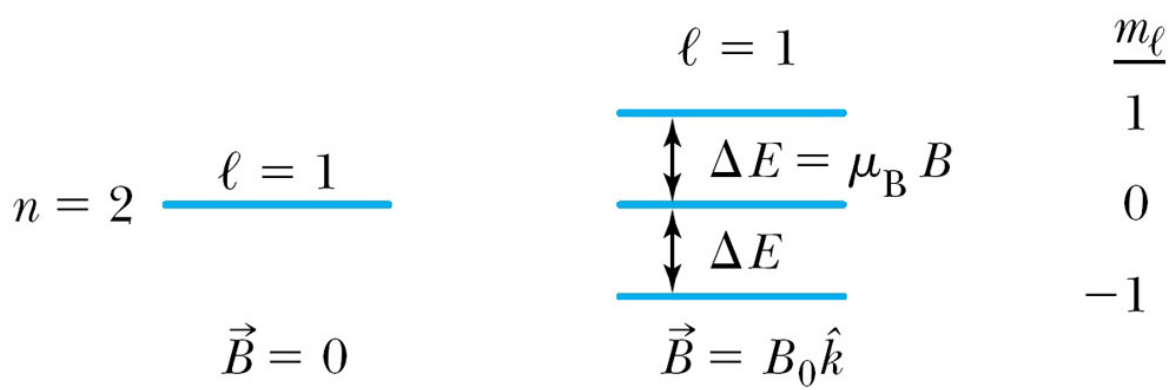
Zeeman effect

- Normal Zeeman effect
  - Magnetic field splits m_l levels
  - Equally spaced energy level ($\Delta E = \mu_B B\, \Delta m_\ell$)
- Anomalous Zeeman effect
  - Electron spin magnetic moment 고려시 발생
  - Normal Zeeman + spin

$$\Delta E = \frac{e}{2m}(\vec{L} + 2\vec{S}) \cdot \vec{B} = g_L \mu_B m_j B$$

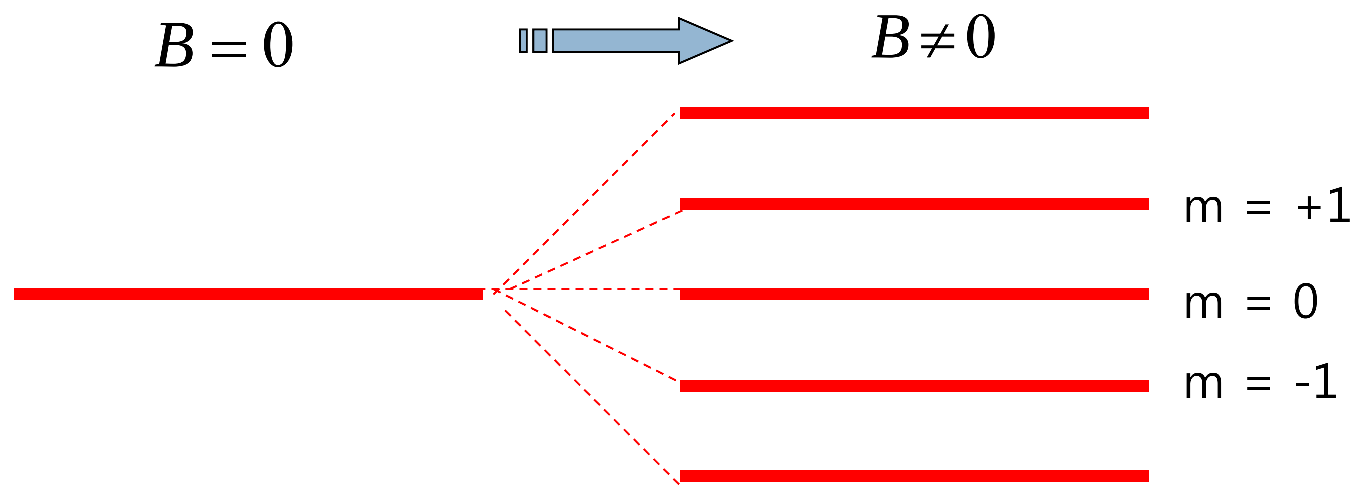
Magnetic interaction energy

m_ℓ	Energy
1	$E_0 + \mu_B B$
0	E_0
−1	$E_0 - \mu_B B$



Magnetic quantum number, m

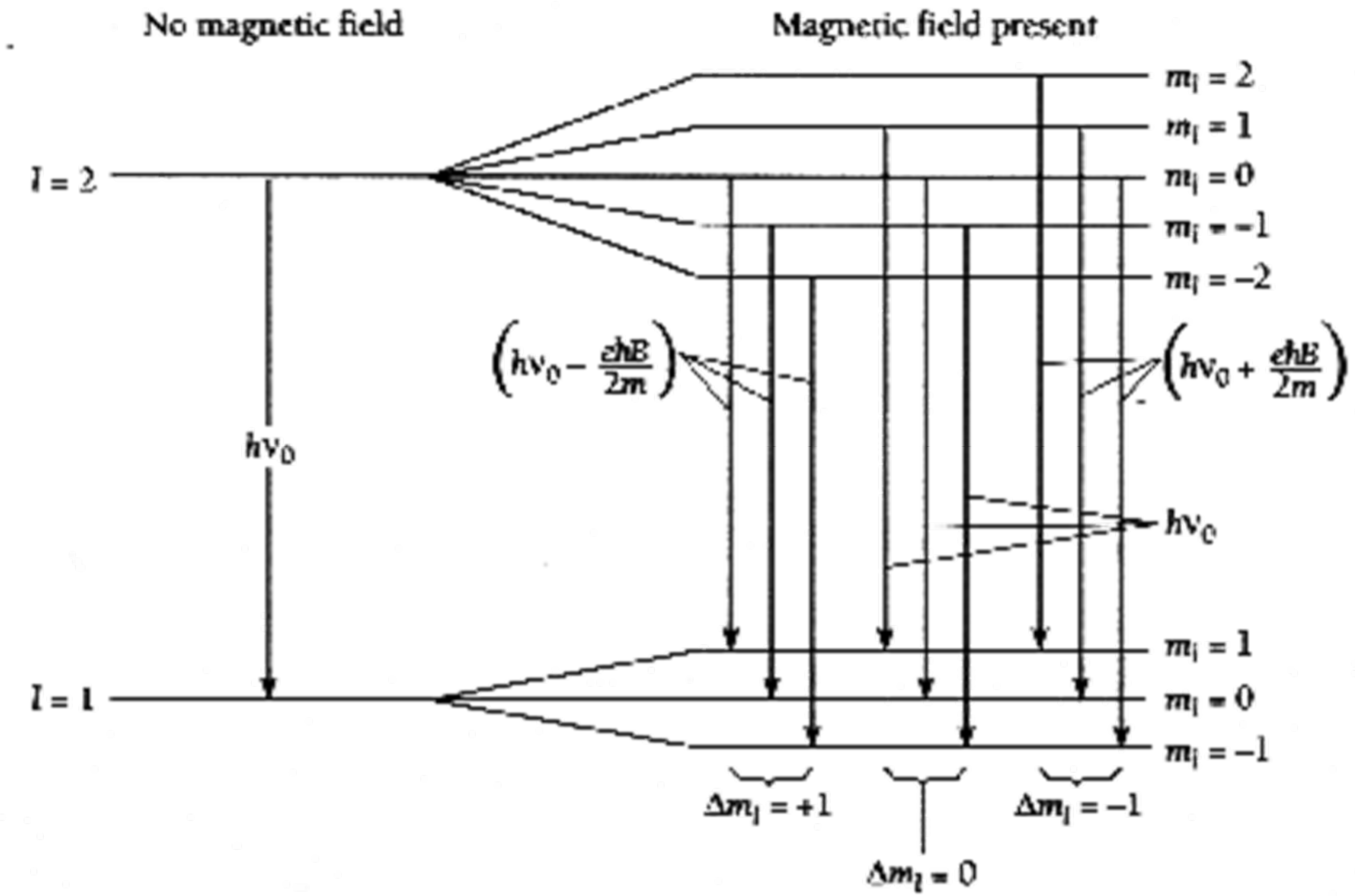
- 자기장에 의한 스펙트럼 추가 분리
  - Orbital orientation을 반영
  - Ground state는 n=1, l=0이므로 m=0으로 분리 안됨



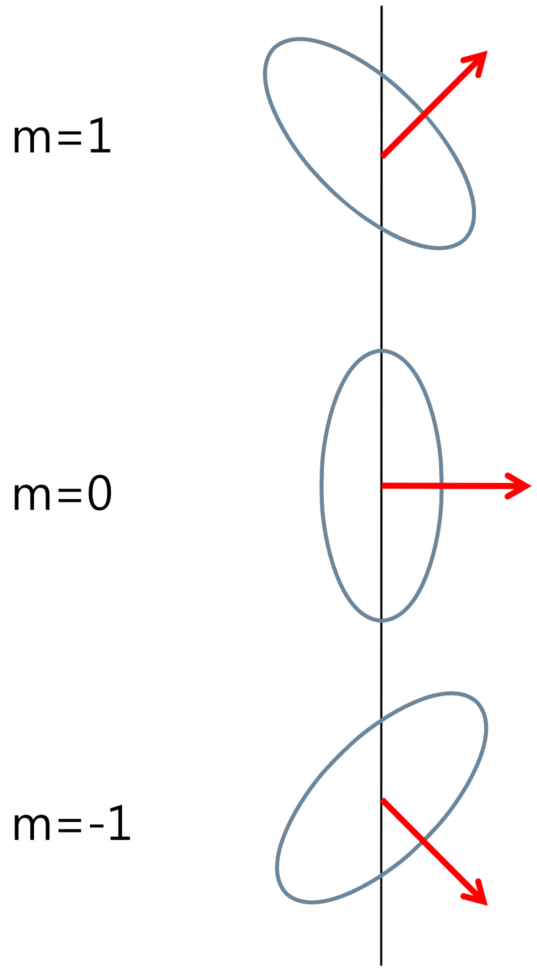
(2l+1) states with same energy: m=-l,…+l

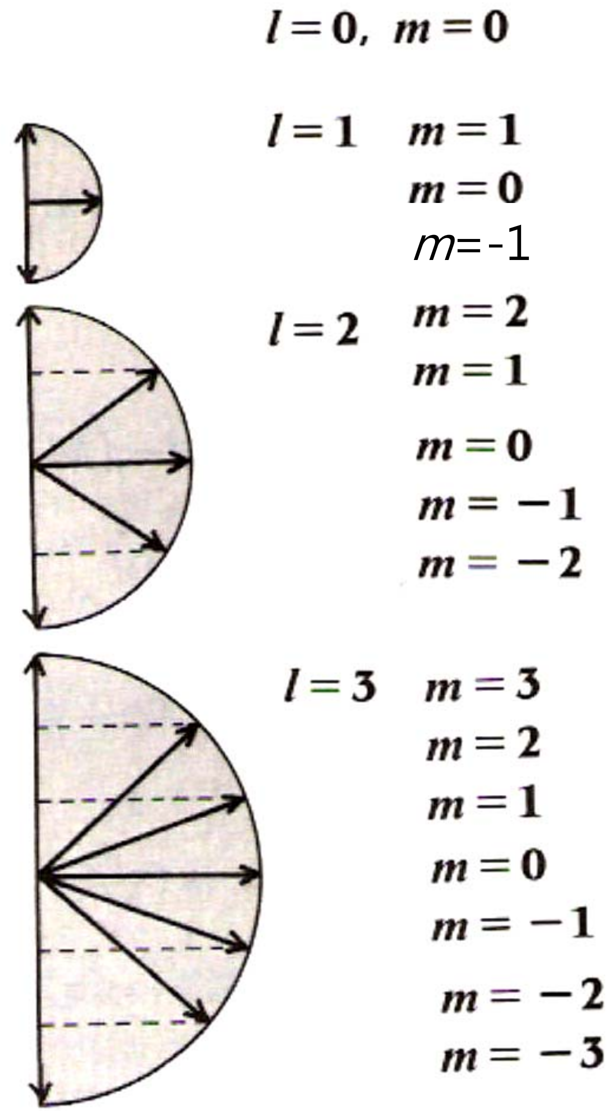
B ≠ 0: (2l+1) states with disti nct energies

전이시 에너지 변화


No magnetic field
Magnetic field present
l = 2
l = 1
hv_0
$m_l = 2$
$m_l = 1$
$m_l = 0$
$m_l = -1$
$m_l = -2$
$\left(hv_0 - \frac{ehB}{2m}\right)$
$\left(hv_0 + \frac{ehB}{2m}\right)$
hv_0
$m_l = 1$
$m_l = 0$
$m_l = -1$
$\Delta m_l = +1$
$\Delta m_l = 0$
$\Delta m_l = -1$

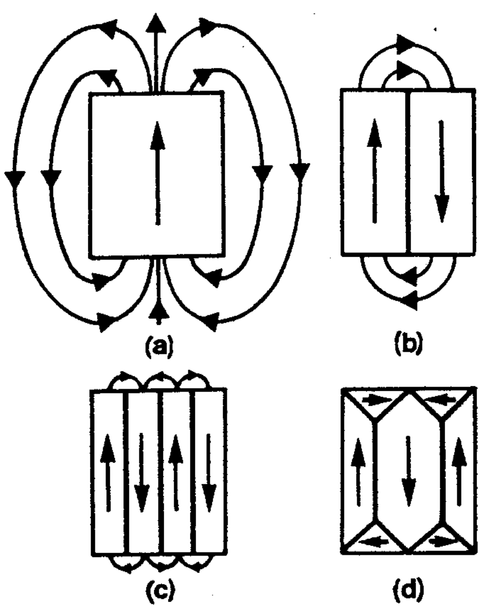
각운동량 벡터 방향과 자기양자수

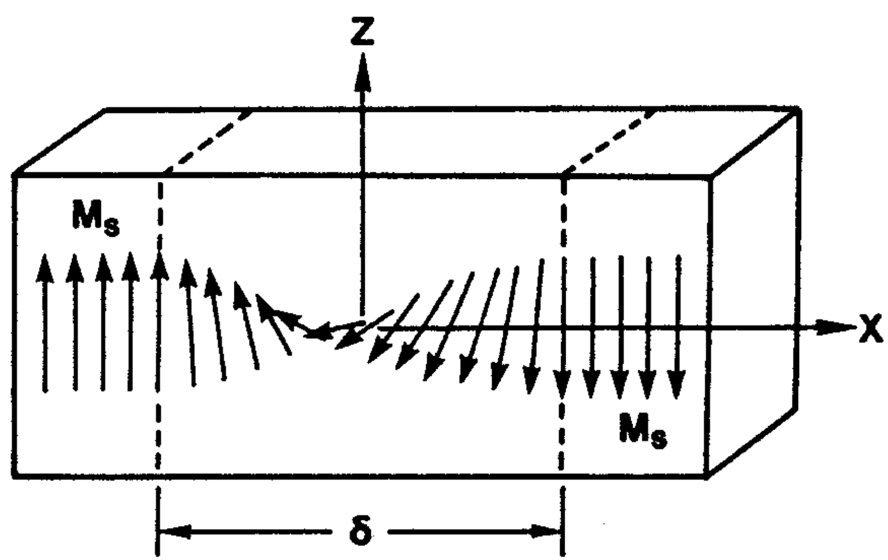




Magnetic domain

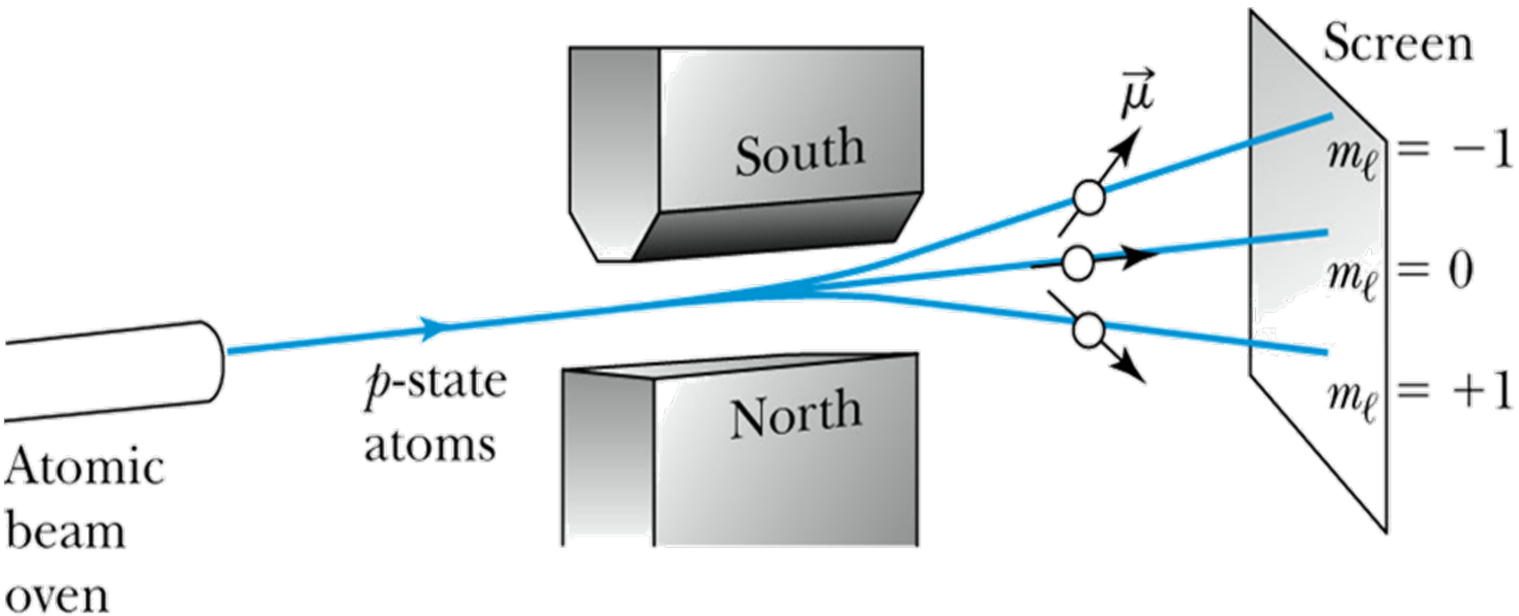
- 자기양자수 발견이 늦은 이유
  - Natural magnetic materials 풍부
  - Magnetic domain의 무작위 배열로 net magnetization 파악 어려움
  - 외부 자기장하에서 분리 가능





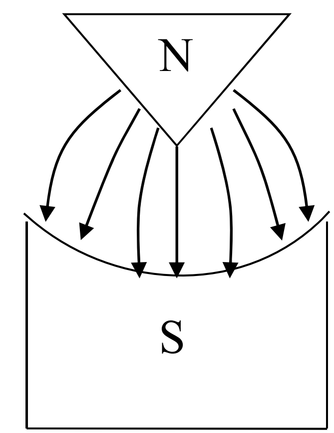
Zeeman effect 실험적 예측

- Stern-Gerlach 실험으로 지만 효과 증명
  - m_ℓ = +1 state: deflected down
  - m_ℓ = -1 state: deflected up
  - m_ℓ = 0 state: undeflected

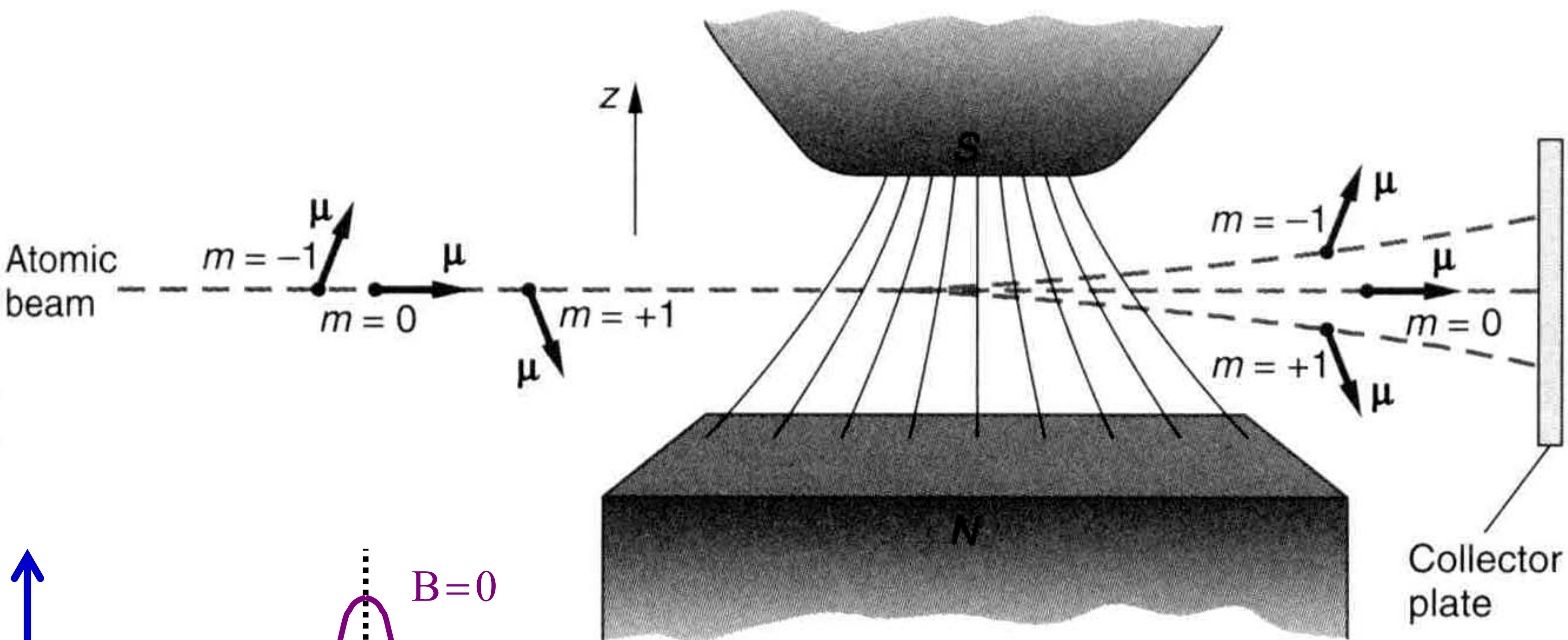


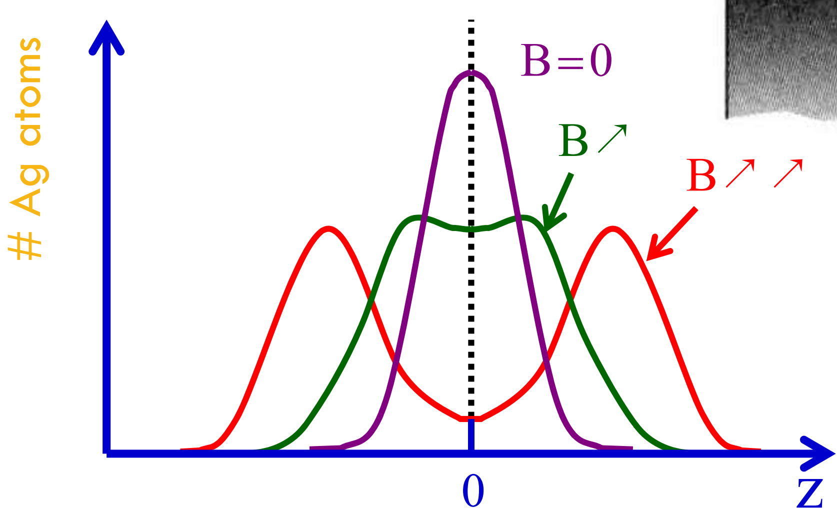
Stern-Gerlach 실험의 의미

- Magnetic force $\left(F_z = \mu_z \dfrac{dB}{dz} \right)$
  - Magnetic moment와 B field gradient에 의존
- 실험 세팅
  - Non-uniform magnetic field 형성
  - Magnetic dipole moment 형성
- Spin의 개념 도출
  - Bohr-Sommerfeld 모델에 의한 2*l*+1 예측
  - Magnetic moment와 orbital angular momentum과의 상관성 설명

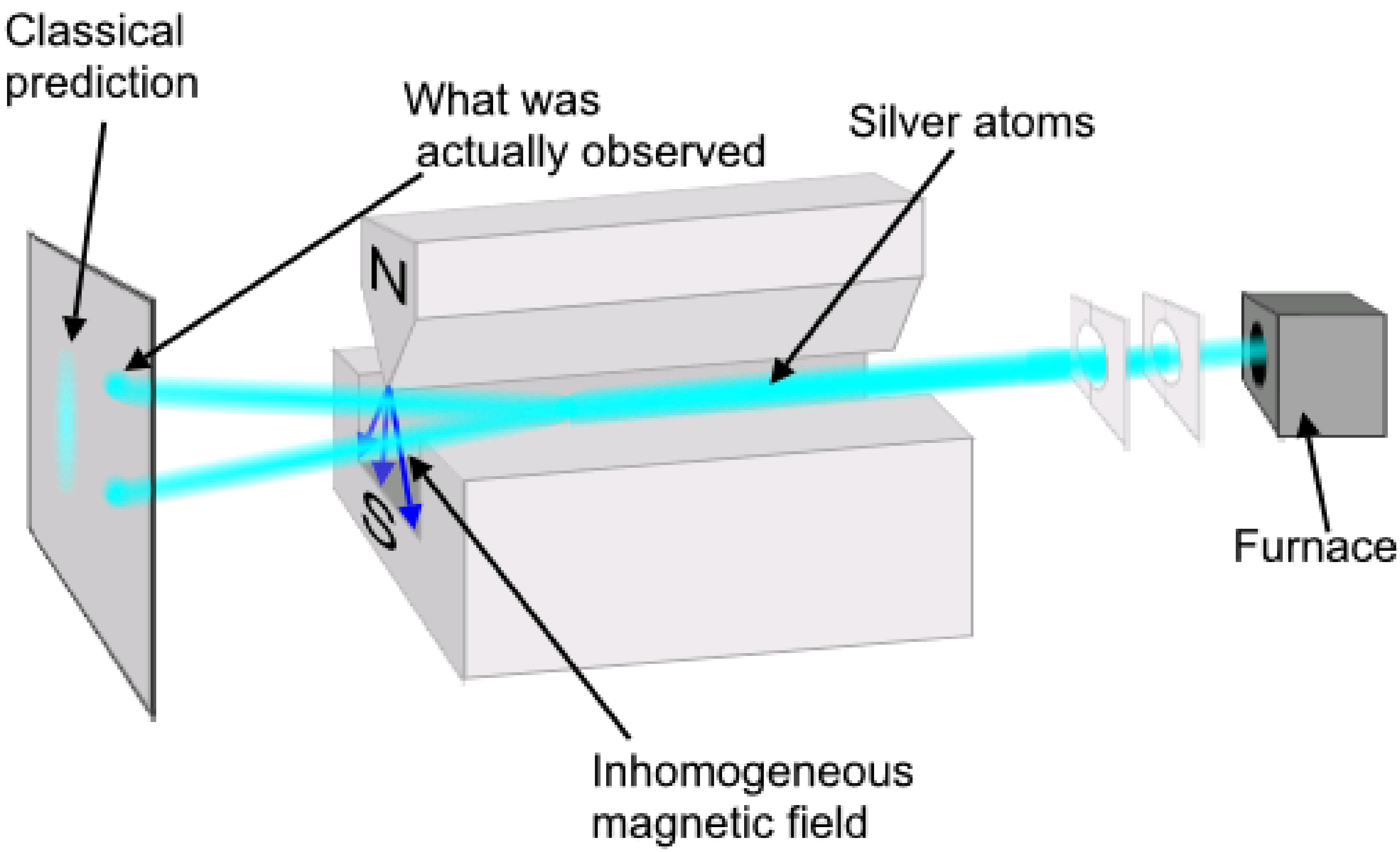


비대칭 자기장 실험 결과





CM 해석과 비교


Classical
prediction
What was
actually observed
Silver atoms
N
S
Furnace
Inhomogeneous
magnetic field