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现代原子物理

SSJ笔记

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PHYS6104P 现代原子物理 **2021-02-20**

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Textbook: *Atomic Physics*, by C. J. Foot, 科学出版社
线上阅读 available online: link

Lectures: Tuesday (3, 4, 5) 09:45 - 12:10, Thursday (6, 7) 14:00 - 15:35 Room 2421
* First class on Tuesday, Mar. 9th.

Homework: 线上提交 Blackboard

- Assignments are uploaded following the lectures on both Tuesday and Thursday, and are due at the beginning (09:45) of the lecture on the following Tuesday.
- Late homework
  - ✧ Homework is not accepted more than one week after its due date.
  - ✧ Late homework is accepted for no more than twice throughout the semester.
- Discussion is encouraged, but copying is regarded as cheating.

Grades: Homework – 40%; Midterm exam – 20%; Final exam – 30%; Presentation – 10%.
开卷，可以带课本或者笔记，很难 | 6月份左右

Topics:

1. The hydrogen atom
2. Multi-electron atoms
3. Interaction: two-level system
4. Magnetic resonance method
5. Interaction: optical excitation
6. Laser control and measurement
7. Doppler-free spectroscopy
8. Laser cooling and trapping
9. Ion trapping
10. Quantum entanglement
11. Atom interferometry
12. Precision spectroscopy for new physics
13. Student presentations

专业内容

Chapter 0 Introduction

1. 原子钟

历史

钟的历史悠久。伽利略发现钟摆。之后，1656年，惠更斯(Chritiaan Huygans)制作了第一个利用钟摆的钟--Pendulum Clock。

1.1 1秒的定义：

```
1967-1968年，1秒的定义是：当铯133原子处于非扰动基态时两个超精细能级间跃迁9192631770次。

1997年补充，在0k条件下。
```

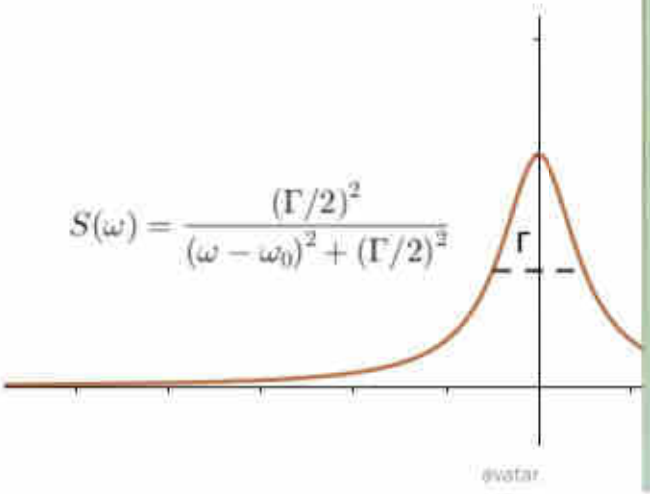
Cs133的基态是 $6^2S_{1/2}$ 与核自旋($I=7/2$)相互作用劈裂成两个能级 $F=3$ 和 $F=4$.

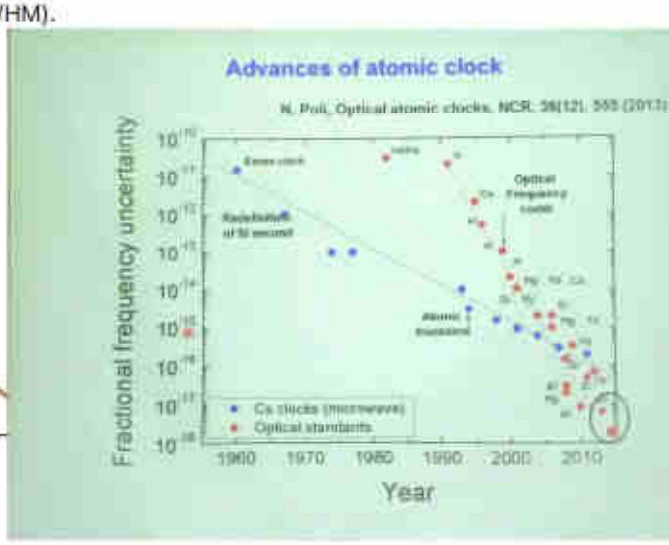
1.2 Lorentzian 分布

这个分布最开始是由Cauchy于17世纪发现的所以也叫做Cauchy分布，或Cauchy-Lorentz分布。它描述了频率的分布：

$$S(\omega)=\frac{(\Gamma/2)^2}{(\omega-\omega_0)^2+(\Gamma/2)^2}$$

在这样的定义下面，我们不妨定义频率的变化范围为： $\delta\omega=\Gamma$ 去描述角频率的不确定度。在图像上，Γ 表达的是半腰全宽(Full Width of Half Maximum, FWHM).





Lorentzian 分布是的逆傅立叶变换为类似于原子衰变的公式（或者说，它是指数下降的傅立叶变换）：

$$S(t)=\exp(-t/\tau),\qquad \tau=1/\Gamma$$

有经验的人，提出的可能性是可靠的，提出的方法是可靠的。但是对于“不可能”往往是不可靠的。阐述“不可靠”这个结论时，往往含有假设在里面。如果试图绕过这个假设或者推翻这个假设，问题有可能被得到解决。

武汉物理与数学研究所，现在叫中科院精密测量科学和技术创新研究院。梅刚华老师，用的铷（Rubidium）元素，放到北斗卫星上面。

稳定度不是与时间成正比，而是与时间的根号成正比。

0.1 Systematic Effect

Systematic Effects

- Zeeman shift
- AC stark shift
- Collisional shift
- Doppler shift
- Time dilation
- Gravitational red shift

在实际的原子钟的测量中，可能无法保证磁场电场等均为零，速度也减不下来。所以最后还是要通过计算把这些效应的影响减掉。

Zeeman Shift: 磁场引起的

AC Stark Shift: 电场引起的

Collisional Shift: 接近的过程中，会相互作用像一个分子一样。造成能级的移动。

Doppler Shift:

Time Dilation: $\frac{\Delta f}{f} = \left(\frac{v}{c}\right)^2 \sim 10^{-12}$ (Room Temperature)

Gravitational Red Shift: $\frac{\Delta f}{f} = \frac{gh}{c^2} \sim 10^{-16}$ (取h=1)

0.2 Formula No.1:

$$\frac{\Delta f}{f} = \frac{1}{f} \frac{1}{\sqrt{N_{atom}\, \tau \cdot T}}$$

Clock Stability

$$\text{Fractional Frequency Stability} \propto \frac{\text{Frequency Error}}{\text{Frequency}}$$

$$\text{Freq Error (stat.)} \propto \frac{1}{\tau} \cdot \frac{1}{\sqrt{N_{atom}}} \cdot \frac{1}{\sqrt{N_{meas}}} \propto \frac{1}{\sqrt{N_{atom} \cdot \tau \cdot T}}$$

T → 总测量时间

τ → 单次测量时间

Allan Deviation $\sigma_y(\tau) = \sqrt{\frac{1}{2(M-1)} \sum_{i=1}^{M-1} (y_{i+1} - y_i)^2}$

Tells the accuracy of atomic clock.

先把总时间分成M-1段，每一段取一个平均值，然后来算。是时间\tau的函数

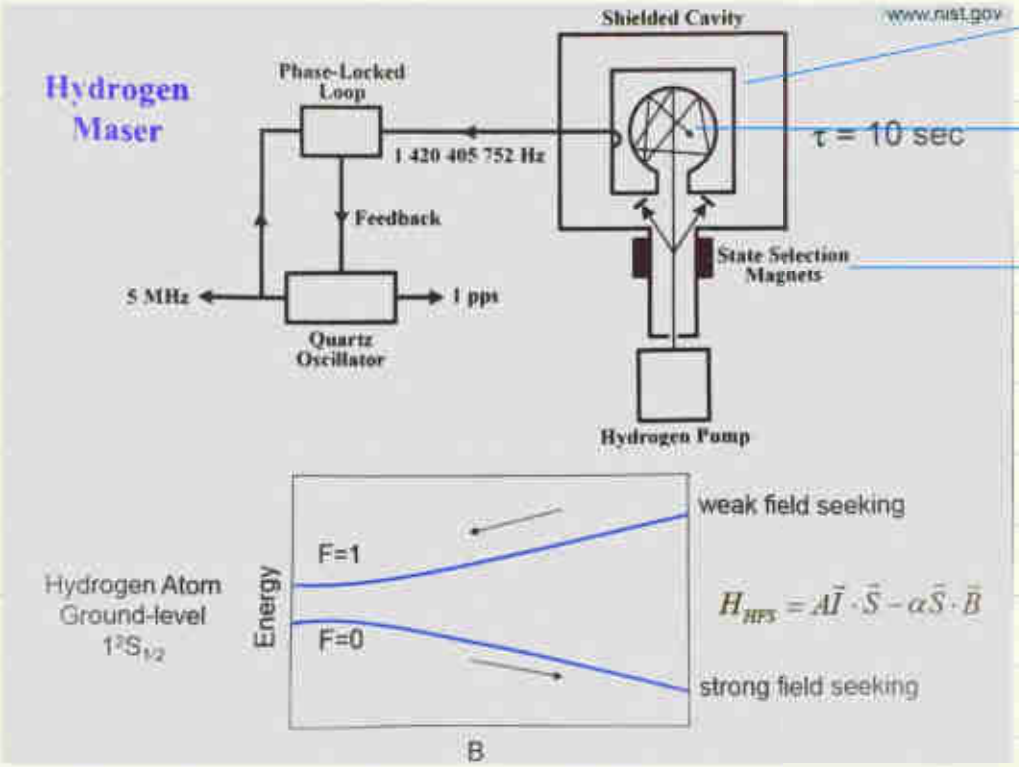
Allan Deviation 是根号 Allan variance。

Allan deviation中的\tau是上面Formula 1里面的T。

0.3 Atomic Clock

几种不同的做钟的办法：

1.Maser：Microwave Amplification by Stimulated Emission of Radiation



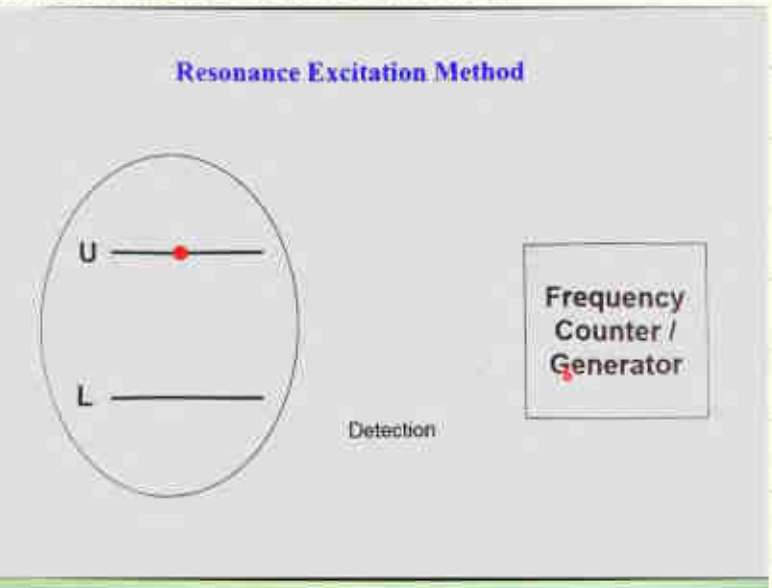
微波腔

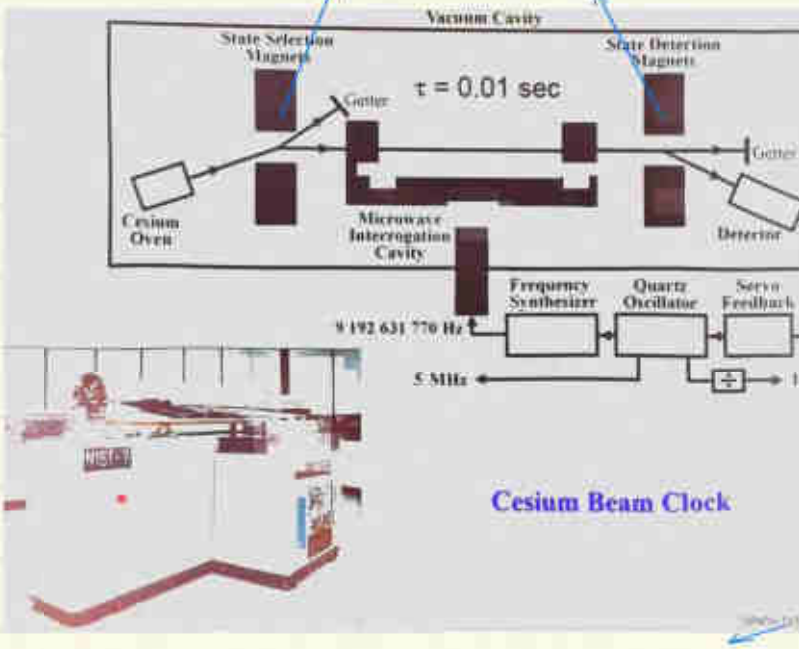
氢原子：这群要求形成一个 population inversion

用塞曼平移的方法（磁场）来行态选择。

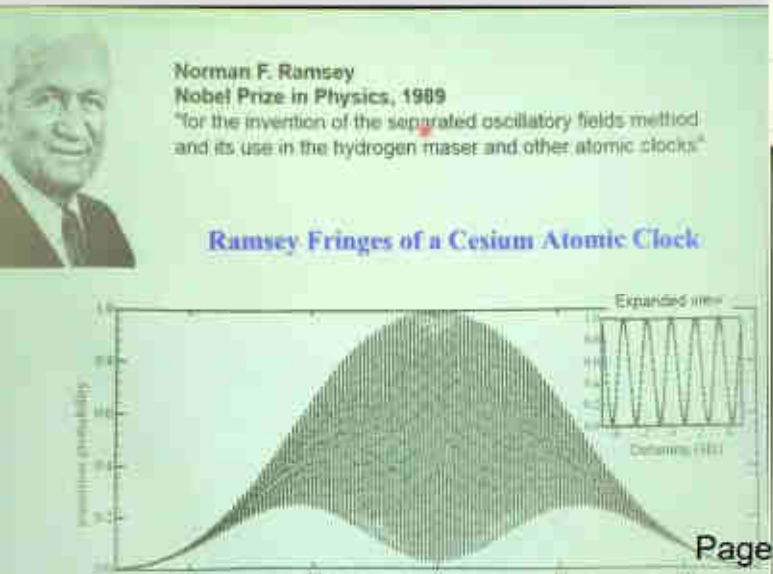
2.Resonance Excitation Method

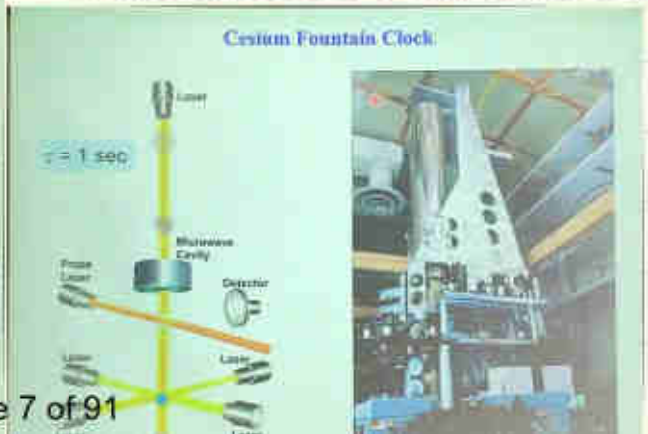
用磁场进行态选择





National Institute of Standards and Technolog





CODATA RECOMMENDED VALUES OF THE FUNDAMENTAL PHYSICAL CONSTANTS: 2018

NIST SP 961 (May 2019)

An extensive list of constants is available on the NIST Physics Laboratory Web site physics.nist.gov/constants. For numerical values a number in parentheses, if present, is the one-standard-deviation uncertainty in the last two digits. For units with square brackets the full descriptions of m^{-1} and m are cycles per meter and meter per cycle, respectively. For the first radiation constant the full description of m^2 is m^{-2} (m/cycle)^4.

Quantity	Symbol	Numerical value	Unit
speed of light in vacuum	c	299 792 458 (exact)	$m\ s^{-1}$
Newtonian constant of gravitation	G	$6.674\,30(15) \times 10^{-11}$	$m^3\ kg^{-1}\ s^{-2}$
Planck constant	h	$6.626\,070\,15 \times 10^{-34}$ (exact)	$J\ Hz^{-1}$
in eV s		$4.135\,667\,696\ldots \times 10^{-15}$	$eV\ Hz^{-1}$
	$\hbar$	$1.054\,571\,817\ldots \times 10^{-34}$	J s
in eV s		$6.582\,119\,569\ldots \times 10^{-16}$	eV s
elementary charge	e	$1.602\,176\,634 \times 10^{-19}$ (exact)	C
vacuum magnetic permeability $4\pi\alpha\hbar/e^2c$	μ_0	$1.256\,637\,062\,12(19) \times 10^{-6}$	$N\ A^{-2}$
$\mu_0/(4\pi \times 10^{-7})$		1.000 000 000 55(15)	$N\ A^{-2}$
vacuum electric permittivity $1/\mu_0c^2$	ε_0	$8.854\,187\,8128(13) \times 10^{-12}$	$F\ m^{-1}$
Josephson constant $2e/h$	K_J	$483\,597.848\,4\ldots \times 10^9$	$Hz\ V^{-1}$
von Klitzing constant $\mu_0c/2\alpha = 2\pi\hbar/e^2$	R_K	25 812.807 45...	Ω
magnetic flux quantum $2\pi\hbar/(2e)$	Φ_0	$2.067\,833\,848\ldots \times 10^{-15}$	Wb
Bohr magneton $e\hbar/2m_e$	μ_B	$9.274\,010\,0783(28) \times 10^{-24}$	$J\ T^{-1}$
in eV T^{-1}		$5.788\,381\,8060(17) \times 10^{-5}$	$eV\ T^{-1}$
nuclear magneton $e\hbar/2m_p$	μ_N	$5.050\,783\,7461(15) \times 10^{-27}$	$J\ T^{-1}$
in eV T^{-1}		$3.152\,451\,258\,44(96) \times 10^{-8}$	$eV\ T^{-1}$
fine-structure constant $e^2/4\pi\varepsilon_0\hbar c$	α	$7.297\,352\,5693(11) \times 10^{-3}$	
inverse fine-structure constant	α^{-1}	137.035 999 084(21)	
Rydberg frequency $\alpha^2m_ec^2/2h = E_h/2h$	cR_∞	$3.289\,841\,960\,2508(64) \times 10^{15}$	Hz
energy equivalent in eV		13.605 693 122 994(26)	eV
Rydberg constant	R_∞	10 973 731.568 160(21)	$[m^{-1}]$
Bohr radius $\hbar/\alpha m_ec = 4\pi\varepsilon_0\hbar^2/m_ee^2$	a_0	$5.291\,772\,109\,03(80) \times 10^{-11}$	m
Hartree energy $\alpha^2m_ec^2 = e^2/4\pi\varepsilon_0a_0 = 2(cR_\infty)h$	E_h	$4.359\,744\,722\,2071(85) \times 10^{-18}$	J
in eV		27.211 386 245 988(53)	eV
electron mass	m_e	$9.109\,383\,7015(28) \times 10^{-31}$	kg
in u		$5.485\,799\,090\,65(16) \times 10^{-4}$	u
energy equivalent in MeV	m_ec^2	0.510 998 950 00(15)	MeV
electron-muon mass ratio	m_e/m_μ	$4.836\,331\,69(11) \times 10^{-3}$	
electron-proton mass ratio	m_e/m_p	$5.446\,170\,214\,87(33) \times 10^{-4}$	
electron charge to mass quotient	$-e/m_e$	$-1.758\,820\,010\,76(53) \times 10^{11}$	$C\ kg^{-1}$
reduced Compton wavelength $\hbar/m_ec = \alpha a_0$	$\lambda\!\!\!^{-}_C$	$3.861\,592\,6796(12) \times 10^{-13}$	m
Compton wavelength	λ_C	$2.426\,310\,238\,67(73) \times 10^{-12}$	[m]
classical electron radius α^2a_0	r_e	$2.817\,940\,3262(13) \times 10^{-15}$	m
Thomson cross section $(8\pi/3)r_e^2$	σ_e	$6.652\,458\,7321(60) \times 10^{-29}$	m^2
electron magnetic moment	μ_e	$-9.284\,764\,7043(28) \times 10^{-24}$	$J\ T^{-1}$
to Bohr magneton ratio	μ_e/μ_B	$-1.001\,159\,652\,181\,28(18)$	
to nuclear magneton ratio	μ_e/μ_N	$-1838.281\,971\,88(11)$	
electron magnetic moment anomaly $\lvert\mu_e\rvert/\mu_B - 1$	a_e	$1.159\,652\,181\,28(18) \times 10^{-3}$	
electron g-factor $-2(1 + a_e)$	g_e	$-2.002\,319\,304\,362\,56(35)$	
electron-proton magnetic moment ratio	μ_e/μ_p	$-658.210\,687\,89(20)$	
muon mass in u	m_μ	0.113 428 9259(25)	u
energy equivalent in MeV	$m_\mu c^2$	105.658 3755(23)	MeV
muon-electron mass ratio	m_μ/m_e	206.768 2830(46)	
muon magnetic moment	μ_μ	$-4.490\,448\,30(10) \times 10^{-26}$	$J\ T^{-1}$
to Bohr magneton ratio	μ_μ/μ_B	$-4.841\,970\,47(11) \times 10^{-3}$	
to nuclear magneton ratio	μ_μ/μ_N	$-8.890\,597\,03(20)$	
muon magnetic moment anomaly			
$\lvert\mu_\mu\rvert/(e\hbar/2m_\mu) - 1$	a_μ	$1.165\,920\,89(63) \times 10^{-3}$	

Quantity	Symbol	Numerical value	Unit
muon g-factor $-2(1 + a_\mu)$	g_μ	$-2.002\,331\,8418(13)$	
muon-proton magnetic moment ratio	μ_μ/μ_p	$-3.183\,345\,142(71)$	
proton mass	m_p	$1.672\,621\,923\,69(51) \times 10^{-27}$	kg
in u		1.007 276 466 621(53)	u
energy equivalent in MeV	m_pc^2	938.272 088 16(29)	MeV
proton-electron mass ratio	m_p/m_e	1836.152 673 43(11)	
proton magnetic moment	μ_p	$1.410\,606\,797\,36(60) \times 10^{-26}$	$J\ T^{-1}$
to nuclear magneton ratio	μ_p/μ_N	2.792 847 344 63(82)	
proton magnetic shielding correction $1-\mu'_p/\mu_p$	σ'_p	$2.5689(11) \times 10^{-5}$	
(H_2O, sphere, 25 °C)			
proton gyromagnetic ratio $2\mu_p/\hbar$	γ_p	$2.675\,221\,8744(11) \times 10^8$	$s^{-1}\ T^{-1}$
		42.577 478 518(18)	$MHz\ T^{-1}$
shielded proton gyromagnetic ratio $2\mu'_p/\hbar$	γ'_p	$2.675\,153\,151(29) \times 10^8$	$s^{-1}\ T^{-1}$
(H_2O, sphere, 25 °C)			
		42.576 384 74(46)	$MHz\ T^{-1}$
neutron mass in u	m_n	1.008 664 915 95(49)	u
energy equivalent in MeV	m_nc^2	939.565 420 52(54)	MeV
neutron-proton mass ratio	m_n/m_p	1.001 378 419 31(49)	
neutron magnetic moment	μ_n	$-9.662\,3651(23) \times 10^{-27}$	$J\ T^{-1}$
to nuclear magneton ratio	μ_n/μ_N	$-1.913\,042\,73(45)$	
deuteron mass in u	m_d	2.013 553 212 745(40)	u
energy equivalent in MeV	m_dc^2	1875.612 942 57(57)	MeV
deuteron-proton mass ratio	m_d/m_p	1.999 007 501 39(11)	
deuteron magnetic moment	μ_d	$4.330\,735\,094(11) \times 10^{-27}$	$J\ T^{-1}$
to nuclear magneton ratio	μ_d/μ_N	0.857 438 2338(22)	
helion (^{3}He nucleus) mass in u	m_h	3.014 932 247 175(97)	u
energy equivalent in MeV	m_hc^2	2808.391 607 43(85)	MeV
shielded helion magnetic moment	μ'_h	$-1.074\,553\,090(13) \times 10^{-26}$	$J\ T^{-1}$
(gas, sphere, 25 °C)			
to Bohr magneton ratio	μ'_h/μ_B	$-1.158\,671\,471(14) \times 10^{-3}$	
to nuclear magneton ratio	μ'_h/μ_N	$-2.127\,497\,719(25)$	
alpha particle mass in u	m_α	4.001 506 179 127(63)	u
energy equivalent in MeV	$m_\alpha c^2$	3727.379 4066(11)	MeV
Boltzmann constant	k	$1.380\,649 \times 10^{-23}$ (exact)	$J\ K^{-1}$
Avogadro constant	N_A	$6.022\,140\,76 \times 10^{23}$ (exact)	mol^{-1}
atomic mass constant $\frac{1}{12}m(^{12}C) = 1$ u	m_u	$1.660\,539\,066\,60(50) \times 10^{-27}$	kg
energy equivalent in MeV	m_uc^2	931.494 102 42(28)	MeV
Faraday constant N_Ae	F	96 485.332 12...	$C\ mol^{-1}$
molar gas constant N_Ak	R	8.314 462 618...	$J\ mol^{-1}\ K^{-1}$
in eV K^{-1}		$8.617\,333\,262\ldots \times 10^{-5}$	$eV\ K^{-1}$
molar volume of ideal gas RT/p	V_m	$22.413\,969\,54\ldots \times 10^{-3}$	$m^3\ mol^{-1}$
(T = 273.15 K, p = 101.325 kPa)			
Stefan-Boltzmann constant $\pi^2k^4/60\hbar^3c^2$	σ	$5.670\,374\,419\ldots \times 10^{-8}$	$W\ m^{-2}\ K^{-4}$
first radiation constant $2\pi hc^2$	c_1	$3.741\,771\,852\ldots \times 10^{-16}$	$[W\ m^2]$
second radiation constant hc/k	c_2	$1.438\,776\,877\ldots \times 10^{-2}$	[m K]
Wien displacement law constant			
$b = \lambda_{max}T = c_2/4.965\,114\,231\ldots$	b	$2.897\,771\,955\ldots \times 10^{-3}$	[m K]
Cu x unit: $\lambda(\text{Cu K}\alpha_1)/1\,537.400$	$xu(\text{Cu K}\alpha_1)$	$1.002\,076\,97(28) \times 10^{-13}$	m
Mo x unit: $\lambda(\text{Mo K}\alpha_1)/707.831$	$xu(\text{Mo K}\alpha_1)$	$1.002\,099\,52(53) \times 10^{-13}$	m

Energy equivalents

$[1\ m^{-1}]c = 299\,792\,458$ Hz	$(1\ Hz)h/k = 4.799\,243\,073\ldots \times 10^{-11}$ K	$(1\ J) = 6.241\,509\,074\ldots \times 10^{18}$ eV	$(1\ eV)/c^2 = 1.073\,544\,102\,33(32) \times 10^{-9}$ u
$[1\ m^{-1}]hc/k = 1.438\,776\,877\ldots \times 10^{-2}$ K	$(1\ Hz)h = 4.135\,667\,696\ldots \times 10^{-15}$ eV	$(1\ eV) = 1.602\,176\,634 \times 10^{-19}$ J	$(1\ kg) = 6.022\,140\,7621(18) \times 10^{26}$ u
$[1\ m^{-1}]hc = 1.239\,841\,984\ldots \times 10^{-6}$ eV	$(1\ K)k/hc = 69.503\,480\,04\ldots\ [m^{-1}]$	$(1\ eV)/hc = 8.065\,543\,937\ldots \times 10^5\ [m^{-1}]$	$(1\ u) = 1.660\,539\,066\,60(50) \times 10^{-27}$ kg
$[1\ m^{-1}]h/c = 1.331\,025\,050\,10(40) \times 10^{-15}$ u	$(1\ K)k/h = 2.083\,661\,912\ldots \times 10^{10}$ Hz	$(1\ eV)/h = 2.417\,989\,242\ldots \times 10^{14}$ Hz	$(1\ u)c/h = 7.513\,006\,6104(23) \times 10^{14}\ [m^{-1}]$
$(1\ Hz)/c = 3.335\,640\,951\ldots \times 10^{-9}\ [m^{-1}]$	$(1\ K)k = 8.617\,333\,262\ldots \times 10^{-5}$ eV	$(1\ eV)/k = 1.160\,451\,812\ldots \times 10^4$ K	$(1\ u)c^2 = 9.314\,941\,0242(28) \times 10^8$ eV

odd字称

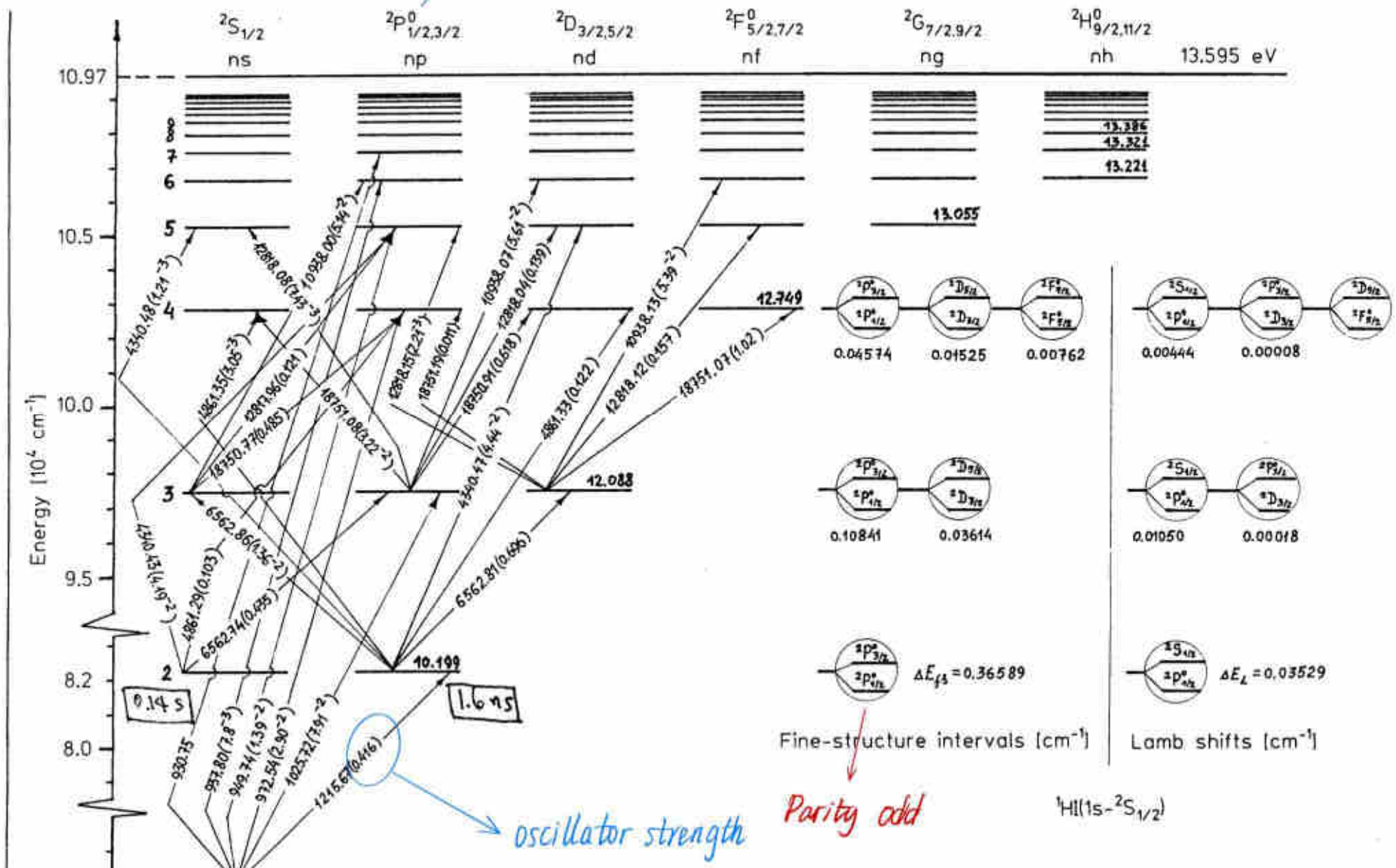


Fig. 7.1. Combined partial energy-level – Grotrian diagram with absorption oscillator strengths for hydrogen

Chapter 1. Hydrogen Atom

1.1 Energy Level of Hydrogen Atom

1885 Balmer 1 Angstrom 一埃 = 0.1nm

1909 Milikan：electron 电的离散

1911 Rutherford 原子核 1e-15: 1fm； 原子 1e-10: 1Angstrom

1913 Bohr $\frac{1}{\lambda} = R\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$ Rydberg constance

$E = hf = h\frac{c}{\lambda} = hc\nu$. $\nu = \frac{1}{\lambda}$ wave number

$n_{air} = 1.0005$ $\lambda_{air} = \frac{\lambda_{vac}}{n_{air}}$

读文献的时候看到波长注意是真空还是空气还是什么介质中的。

Bohr Model

① $m\omega^2 r = \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r^2}$ 认为这三个频率相等是根据经典电动力学理论。

② $\hbar\omega_{nm} = Rhc\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$

③ Corresponding Principle：当n很大，就可用经典电动力学算：

$\underset{n\to\infty}{\lim}$： $\omega_{classical} = \omega_{n+1} - \omega_n$

这样多一个关系式子，把R视为未知数，就把没解释过的物理常数R用其他的物理常数表示出来。找物理常量之间的关系，来解读这个世界。

$\Rightarrow cR_\infty = \frac{\alpha^2 m_e c^2}{2h}$, $\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c}$ Fine Structure Constant

$\Rightarrow r_n = n^2 a_0$, $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$ Bohr radius

$v_n = \frac{1}{n}\alpha c$

$E_n = -hcR\frac{1}{n^2}$

基本常数：定义了光速，从而放弃了米；定义了普朗克常数，从而放弃了质量的定义

Atomic Units：放弃了时间长度质量电荷，定义： $\hbar = 1$, $m_e = 1$, $e = 1$, $\frac{1}{4\pi\varepsilon_0} = 1$

$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r} \xrightarrow{\text{Atomic Units}} \hat{H} = -\frac{\nabla^2}{2} - \frac{1}{r}$

前缀			
	s	second	10^0
	ms	milli second	10^{-3}
	μs	microseond	10^{-6}
	ns	nanosecond	10^{-9}
	ps	picosecond	10^{-12}
	fs	femtosecond	10^{-15}
	as	atto second	10^{-18}

email里面要打micro，不然会变

阿秒

Hz		10^0
KHz	kilo	10^3
MHz	mega	10^6
GHz	giga	10^9
THz	tera	10^{12}

20210316 Tuesday

Bohr推导时，Correspondence Principle是比较有道理的；

而角动量的量子化的这个推导是错误的，首先用一个平面上的轨道来说一个空间的东西不靠谱；另一方面，事实上角动量在z轴上的分量是量子化的，对应的量子数是m而不是n。

严格的推导，用薛定谔方程。
（很幸运的一个事情是，原子是一个球，求解相关问题的时候，使用球坐标。）

$\psi = R_{nl}(r)\, Y_{lm}(\theta, \varphi)$

只有在库伦场中，才有关系：
$$\begin{cases} n = 0, 1, \cdots \\ l = 0, 1, 2, 3, \cdots, n-1 \end{cases}$$
s p d f

$$m = -l, -l+1, \cdots, l$$

Table 2.2 Radial hydrogenic wavefunctions $R_{n,l}$ in terms of the variable $\rho = Zr/(na_0)$, which gives a scaling that varies with n. The Bohr radius a_0 is defin eqs 1.46.

$$R_{1,0} = \left(\frac{Z}{a_0}\right)^{3/2} 2e^{-\rho}$$
$$R_{2,0} = \left(\frac{Z}{2a_0}\right)^{3/2} 2(1-\rho)e^{-\rho}$$
$$R_{2,1} = \left(\frac{Z}{2a_0}\right)^{3/2} \frac{2}{\sqrt{3}}\rho e^{-\rho}$$
$$R_{3,0} = \left(\frac{Z}{3a_0}\right)^{3/2} 2\left(1-2\rho+\frac{2}{3}\rho^2\right)e^{-\rho}$$
$$R_{3,1} = \left(\frac{Z}{3a_0}\right)^{3/2} \frac{4\sqrt{2}}{3}\rho\left(1-\frac{1}{2}\rho\right)e^{-\rho}$$
$$R_{3,2} = \left(\frac{Z}{3a_0}\right)^{3/2} \frac{2\sqrt{2}}{3\sqrt{5}}\rho^2 e^{-\rho}$$

Normalization: $\int_0^\infty R_{n,l}^2\, r^2\, dr = 1$

$$\begin{cases} \text{势能} \quad V^{3d} = -\dfrac{e^2}{4\pi\varepsilon_0}\dfrac{1}{r} \\ (\text{有效势能}) \quad V^{1d} = -\dfrac{e^2}{4\pi\varepsilon_0}\dfrac{1}{r} + \dfrac{\hbar^2}{2m_e}\dfrac{l(l+1)}{r^2} \end{cases}$$

这一项可以解释 $\begin{cases} R_{n0}(r=0) \neq 0 \\ R_{nl}(r=0) = 0, \quad l \neq 0 \end{cases}$

跃迁的选择定则，是由角分布函数决定的。

$Y_{lm}(\theta,\varphi)$ Spherical Harmonic

形成一个完备函数系：

$$f(\theta,\varphi) = \sum_{lm} a_{lm} Y_{lm}(\theta,\varphi)$$

$$\begin{cases} \text{Normalized} & \int |Y_{lm}|^2 d\Omega = 1 \\ \text{Orthogonal} & Y^*_{lm'}(\theta,\varphi)\, Y_{lm}(\theta,\varphi)\, d\Omega = \delta_{ll'}\delta_{mm'} \end{cases}$$

$$Y_{0,0} = \sqrt{\frac{1}{4\pi}}$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta \propto \frac{z}{r}$$

$$Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi} \propto \frac{x\pm iy}{r}$$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$Y_{2,\pm1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}$$

$$Y_{2,\pm2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}$$

Normalisation: $\int_0^{2\pi}\int_0^{\pi} |Y_{l,m}|^2 \sin\theta\, d\theta\, d\phi = 1$

需要会反推，从直角坐标推导球坐标，在后面选择定则会用到。

$$z \sim r Y_{00}, \quad x \sim r(Y_{11} + Y_{1,-1}), \quad y \sim r(Y_{11} - Y_{1,-1})$$

$$\begin{cases} l=1 \text{ 的粒子，称 vector boson （如光子）}, Y_{1m} \\ \text{scalar} \quad Y_{00} \\ \text{tensor of rank 2} \quad Y_{2m} \end{cases}$$

$$Y_{lm}(\theta,\varphi+\pi) = Y_{lm}(\theta,\varphi)\, e^{im\pi}$$

Parity: Spatial inversion symmetry: $(x,y,z) \to (-x,-y,-z)$

$(\theta,\varphi) \to (\pi-\theta, \varphi+\pi)$

也可以通过一次旋转加镜像操作达到反演的目的。

Mirror reflection: $(x,y,z) \to (x,y,-z)$

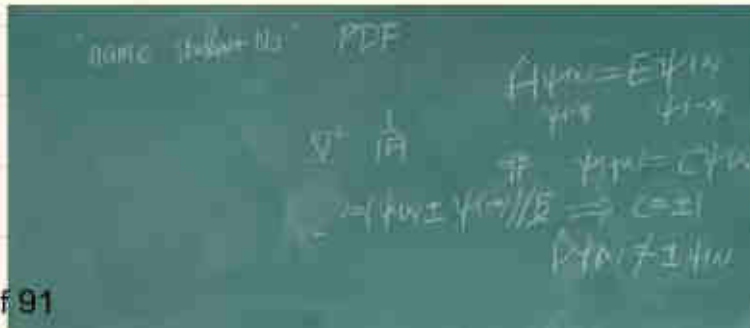
做了Parity这个变换之后：

如果不变就称为是even： 球谐函数 l even

如果变一个符号就是odd： l odd

也存在没有Parity的，比如球谐函数的奇偶叠加。但这必然不是能量的本征态。

符号：如果一个态右上角有一个小圆圈，就是宇称的odd。



1.2 isotope shift

(1) 质量效应: (mass shift)

$$\hat{H} = \frac{p_e^2}{2m_e} + \frac{p_N^2}{2m_N} + V \quad , \quad \vec{p}_e + \vec{p}_N = 0$$

$$= \frac{p_e^2}{2m_e}\left(1 + \frac{m_e}{m_N}\right) + V$$

$$= \frac{p_e^2}{2\mu} + V \, , \qquad \mu = \frac{m_e m_N}{m_e + m_N}$$ ，把电子质量变小了

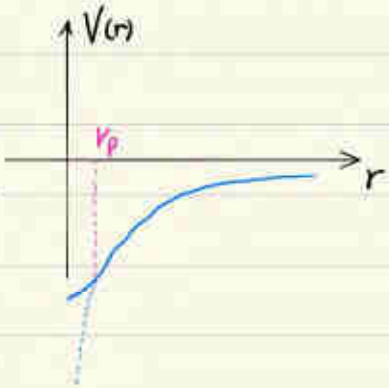
$$R_\infty \to \left(\frac{1}{1+\frac{m}{M}}\right) R_\infty \approx \left(1 - \frac{m}{M}\right) R_\infty$$

频率相差， $f_A - f_{A'} \propto \left(\frac{1}{A} - \frac{1}{A'}\right)$ 对复杂原子也成立。

(2) 核的大小效应:
(Volume shift/field shift) 用一个简单的模型计算：核是一个电荷密度均匀的球形。

① outside $r > r_p$, $V \propto -\frac{1}{r}$

② inside $r < r_p$, $V \propto r$



只对s轨道有影响，s轨道的能级会被抬高。因为s能进入中心。而对后面的p，d等轨道没有影响。所以s到其他的轨道的跃迁谱线能量会减小。

Hydrogen-like

Positronium 电子偶素 e^+e^-

Muonium μ^+e^-

Muonic Hydrogen $p^+\mu^-$ Volume shift 效应特别明显。可以通过这个测量质子半径。

1.3 Fine Structure

2.7 Dirac方程

对于1/2自旋的粒子可以用Dirac方程进行描述。当我们转换成普通的哈密顿量的时候，会多出一些项，可以视为相对论修正：

$$\hat{H} = \frac{p^2}{2m} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} - \frac{p^4}{8m^3c^2} + \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}L\cdot S + \frac{\pi\hbar^2}{2m^2c^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)\delta(r)$$

除了前两项表达了基础的部分外，第三项表达了动量更精细的部分，第四项表达了自选轨道耦合，第五项是达尔文项(Darwen term)

Dirac 方程 $i\hbar\gamma^\mu\partial_\mu\psi = mc\psi$, $\mu = 0,1,2,3$

$$\gamma^0 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \qquad \gamma^{1,2,3} = \begin{pmatrix} 0 & \sigma_{x,y,z} \\ -\sigma_{x,y,z} & 0 \end{pmatrix}$$

从公式里面可以推断出有另外一种粒子，质量和自旋和电子一样，而电荷相反。

起名字叫positron.

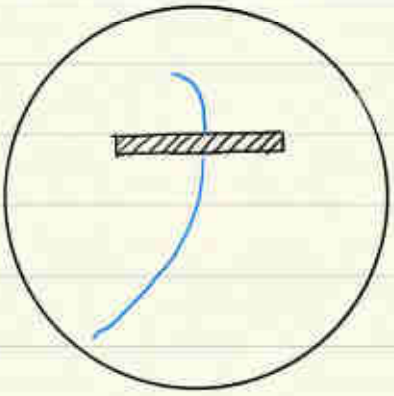
$$m_{e^+} = m_{e^-}$$

$$S_{e^+} = S_{e^-} = \frac{1}{2}\hbar$$

$$q_{e^+} = -q_{e^-}$$

Cloud Chamber

放置一个膜，可以给电子减速。这样就可以判断粒子从上往下运动，还是从下往上。



自旋定义：$\phi \to \phi + 2\pi$

$e^{im\varphi} \to e^{i(m\varphi + m\cdot 2\pi)}$, 电子 $m = \frac{1}{2}$

对电子，得“转动”720度才能回到自己。

$$H = \frac{\vec{p}^2}{2m} - \underbrace{\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}}_{V(r)} - \frac{p^4}{8m^3c^4} + \underbrace{\frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\vec{L}\cdot\vec{S}}_{\text{Spin-orbit coupling, fine structure}} + \frac{\pi\hbar^2}{2m^2c^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)\delta(\vec{r})$$

Darwin

精细结构分裂不会变的：

1. multiplicity
2. center of gravity

例 $n=2,\ l=1,\ s=\frac{1}{2}$

$$\underset{(2l+1)(2s+1)=6}{\underline{P}} \quad \begin{cases} 2^2P^0_{\frac{3}{2}} & 2j_2+1 = 4个 \\ 2^2P^0_{\frac{1}{2}} & 2j_1+1 = 2个 \end{cases}$$

分裂与束缚能之比：$\frac{\Delta E}{E} \sim \alpha^2$, $\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c}$

衡量电磁相互作用的耦合强度

$$\Delta E_{rel} = \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)E_n$$ 与l没关系.

考虑到Dirac方程的解，能量可以表达为：

$$E_{nj} = E_n\left[1 + \frac{(Z\alpha)^2}{\ldots}\left(\frac{n}{\ldots} - \frac{3}{\ldots}\right)\right] + O(Z^2\alpha^2)$$

有相同的能量，同时，上式小量成立的条件是：$Z\alpha < 1$. 我们正在探索原子量大于137的物
同时，我们可以看到精细结构的能量比为：

1.4 Lamb Shift

$S_{\frac{1}{2}}$ _____

$P_{\frac{1}{2}}$ _____

$\vec{\mu}_L = -g_L \mu_B \frac{\vec{L}}{\hbar}$, $g_L = 1$, $\mu_B = \frac{e\hbar}{2m_e}$. Bohr magneton

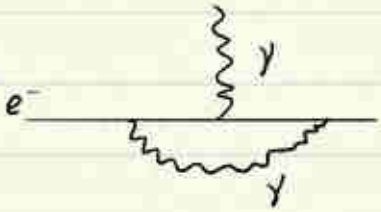
$\vec{\mu}_S = -g_S \mu_B \frac{\vec{S}}{\hbar}$, $g_S = 2$

而实验测量： $g_S = 2 + \frac{\alpha}{\pi}$

Dirac方程无法解释： 1. Lamb移位

2. g_s与2的偏差

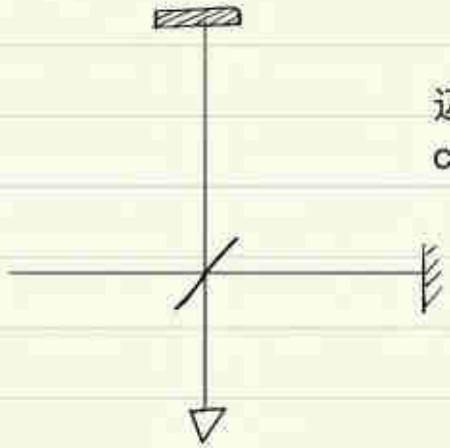
于是有了QED：量子电动力学。



20210323 Tuesday

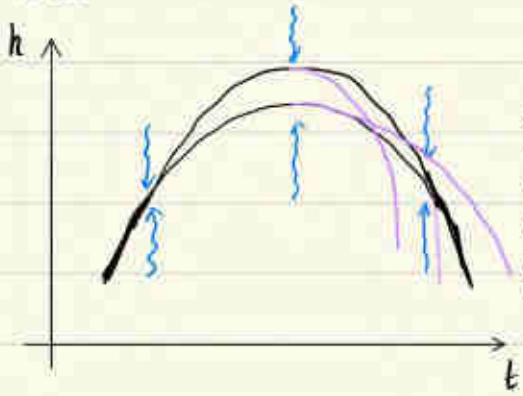
重力加速度的测量

1. 经典



迈克耳孙干涉仪，让上面的镜子（事实上是corner cube）自由落体。

2. 原子干涉仪 atom interferometer



本质上是原子与自己的干涉。原子被第一束光打到之后形成叠加态，同时走上下两条路径。中间的光是为了让两个路径相交。浅蓝色的线是不用的原子的路径。

莫比乌斯带可以和自旋1/2相对应起来，走一圈不能回到原点，必须走两圈。

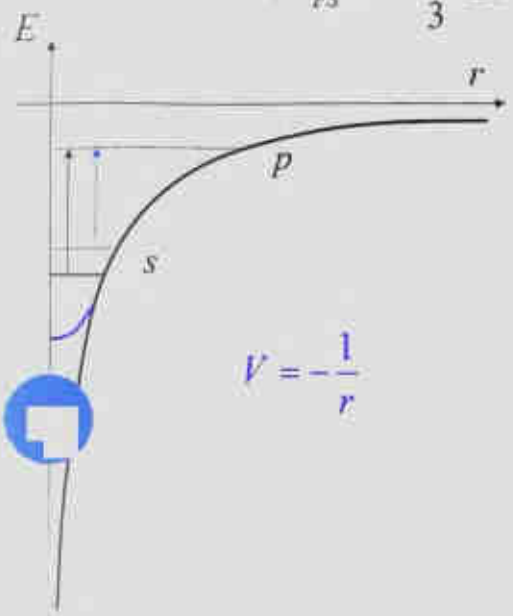
Nuclear Volume Effect 指上下两能级的差

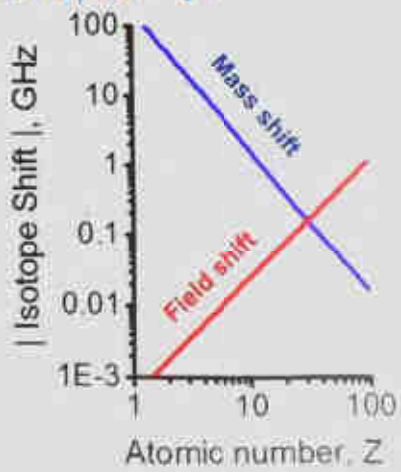
$$\delta\nu_{FS} = -\frac{2\pi}{3} Ze^2 \cdot \Delta|\Psi(0)|^2 \cdot \delta\langle r^2\rangle$$

mean square radius

指两个同位素

$$\langle r^2 \rangle = \int r^2 \rho(r)\, d\Omega$$





而一般的RMS radius指的是 root mean square radius $\sqrt{\langle r^2 \rangle}$

Lamb shift $2^2P_{\frac{1}{2}} - 2^2S_{\frac{1}{2}}$

(1) vacuum fluctuation

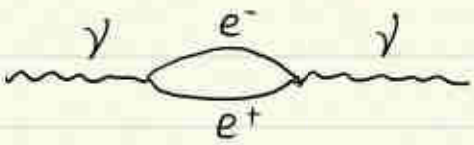
可以控制真空涨落。例如加两面镜子，就可以调控可能产生的涨落。（电磁场总要满足边界条件）

Purcell effect 可以让自发辐射变得慢，也可以让它变快。如果把镜子之间的距离调节正好和跃迁的频率共振，自发跃迁就会发生很快。

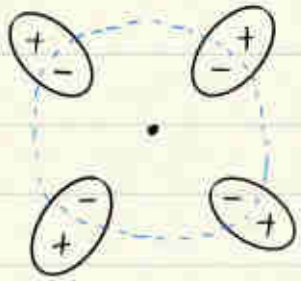
涨落的电磁场会和电子发生作用，然后电子形成一个球，相当于电子的分布密度变了，相应的势能表达式也变了。不能简单写为反比于r。

(2)vacuum polarization

真空不仅能产生光子，还能产生电子（为了保证电荷守恒等，一次出来一个正电子一个电子，然后很快湮灭）



如果在原子核附近发生这种效应，由于原子核带正电荷，会有分布：



整个真空被原子核“极化”了。越接近原子核，效应越显著。

上面两个效应对能级的shift（即这个Lamb Shift）作用是相反的。所以有时候P在S上面，有时候S在P轨道上面。对于氢原子的n=2是S在上面的。

首先，真空具有真空扰动，它有多个效果。首先是，激发态能级的自发跃迁。激发态能级也是稳定的能级，受到跃迁频率的真空扰动的影响，自发跃迁。

第二，真空极化的影响。

（1） $Q < Q_p$ Qp是裸质子电荷，Q是观察到的电荷，显然 $Q = e$，Qp的测量方法由Freeman Deson 给出。

（2）Hawking 辐射。光子会变成一对正负电子然后再湮灭成为光子。当这一过程发生在视界边缘，一部分电子不能出来，另一部分辐射出去，辐射的能量来自于黑洞。

在p-e结果中，在2s和2p能级中，由于volumn effect，2s能级能量要高于2p能级。2s能级在r=0处概率不为0，因此会受到原子核大小的影响，原子核是有限大小的，所以会提高2s能级。同时，会受到兰姆位移的影响。

$$V(r) \to V(r + \delta r)$$

这是在平衡点附近瞬间的位移，它是各个方向的。兰姆位移使得2s能级低于2p能级。对于电子而言（电子质量很小），兰姆位移的影响小于原子核体积的影响。因此，总的影响仍然是2s能级高于2p能级。

但是，对于 $p - \mu$ 对而言，muon是质量更大的“电子”（轻子）。2p能级比2s能级更高。

Chapter 2. Transition

2.1 Angular Momentum

角动量和动量之间一个最大的区别，是对易关系：

$$[\hat{p}_x, \hat{p}_y] = 0 \qquad [\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$$

在做平移的时候，有3个自由度。而在描述旋转的时候，只有2个自由度。

如果发生绕着x的转动以及绕y转动，并不能保证绕z轴不转。

并且由于不对易的影响，有限转动之间并不能交换。

$$\begin{cases} \hat{J}^2 |j, m_j\rangle = j(j+1)\hbar^2 |j, m_j\rangle \\ \hat{J}_z |j, m_j\rangle = m_j \hbar |j, m_j\rangle \\ \hat{J}_\pm |j, m_j\rangle = \sqrt{j(j+1) - m(m\pm1)}\,\hbar\, |j, m_j \pm 1\rangle \end{cases}$$

raising operator / lowing operator

角动量的耦合

以氢原子：$^2S_{\frac{1}{2}}$，$l=0$，$s=\frac{1}{2}$ $\Big\}\, j=\frac{1}{2}$，$I=\frac{1}{2}$ $\Big\}\, F=0,1$

$\vec{F} = \vec{I} + \vec{S}$，$m_F = m_I + m_S$，$F_{max} = I+S$，$F_{min} = |I-S|$

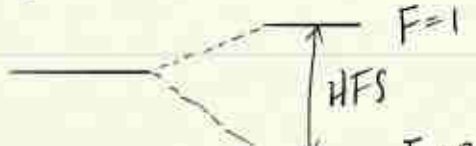
耦合表象	无耦合表象
$\lvert s, m_s, I, m_I\rangle$	$\lvert S\ I\ F\ m_S\rangle$
$\lvert +,+\rangle$	$\lvert 1, 1\rangle$
$\lvert +,-\rangle$	$\lvert 1, 0\rangle$
$\lvert -,+\rangle$	$\lvert 1, -1\rangle$
$\lvert -,-\rangle$	$\lvert 0, 0\rangle$

推导CG系数： Clebsch-Gordon coefficient

$$\left.\begin{aligned} |1,1\rangle &= |+,+\rangle \\ |1,-1\rangle &= |-,-\rangle \end{aligned}\right\} \text{（由 } m_F = m_I + m_S \text{ 保证）}$$

$$\left.\begin{aligned} \hat{F}_- |1,1\rangle &= \sqrt{2}\, |1,0\rangle \\ (\hat{S}_- + \hat{I}_-)|+,+\rangle &= |-,+\rangle + |+,-\rangle \end{aligned}\right\} \Rightarrow |1,0\rangle = \frac{1}{\sqrt{2}}(|+,-\rangle + |-,+\rangle)$$

$|0,0\rangle$ 根据正交性，是 $|0,0\rangle = \frac{1}{\sqrt{2}}(|+,-\rangle - |-,+\rangle)$



（也可以用不管是升算符还是降算符，作用在$|0,0\rangle$上都会得到0来推导系数）

$$|J, m_j, j_1, j_2\rangle = \sum_{m_1 m_2} C_{m_1 m_2} |j_1, m_1, j_2, m_2\rangle$$

CG系数表中有为0的项。对应禁戒的跃迁。有对应的对称性的解释。

举例：1与1的耦合中：

$$|1,0\rangle = \frac{1}{\sqrt{2}}|1,1\rangle|1,-1\rangle + 0|1,0\rangle|1,0\rangle - \frac{1}{\sqrt{2}}|1,-1\rangle|1,1\rangle$$

做镜面反射变-1　　镜面反射不变

$$C_{m_1 m_2} = \langle j_1 m_1 j_2 m_2 | j_1 j_2 J M\rangle$$
$$= (-1)^{J-j_1-j_2} \langle j_2 m_2 j_1 m_1 | j_2 j_1 J M\rangle$$

根据这个式子也可以解释上面的系数是0。

系数是转动时，$e^{-i m_j \pi} = (-1)^{m_j}$

为了完成交换，需要两个先绕着耦合的总角动量的轴转一个pi，再反着绕自己的轴转pi

对称性更高的符号：Wigner's 3j

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-1)^{j_1-j_2-m_3}}{\sqrt{2j_3+1}} \langle j_1 m_1 j_2 m_2 | j_1 j_2 j -m_3\rangle$$

要求 $m_1+m_2+m_3=0$ ，$\Delta(j_1 j_2 j_3)$ （可以构成三角形）

性质：(1) exchange property $\begin{pmatrix} 1 & 2 & 3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} 2 & 1 & 3 \end{pmatrix}$

(2) rotation property $\begin{pmatrix} 1 & 2 & 3 \end{pmatrix} = \begin{pmatrix} 3 & 1 & 2 \end{pmatrix}$

(3) reflection property $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}$

宇称不是角动量本身的性质，还要看某个特定的角动量对应的物理意义。如果只告诉J=1，而m_j=0，并不能确定它的宇称是even还是odd。

只对单电子的轨道角动量成立：　L odd → parity odd -1

L even → parity even 1

而对于复合的角动量：　$\left.\begin{matrix} l_1 = 1 \\ l_2 = 1 \end{matrix}\right\}$ $L = 0, 1, 2$ 都是偶的.

3-j表示和球谐函数的关系

$$\int Y_{l_1 m_1}(\theta,\varphi) Y_{l_2 m_2}(\theta,\varphi) Y_{l_3 m_3}(\theta,\varphi) \sin\theta \, d\theta \, d\varphi$$
$$= \sqrt{\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

5.5 CG系数与球谐函数的关系

（参考 en.wikipedia.org/wiki/C ...）

$$\int_{4\pi} Y_{\ell_1}^{m_1*} Y_{\ell_2}^{m_2*} Y_L^M \, d\Omega = \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2L+1)}} \langle \ell_1\, 0\, \ell_2\, 0 | L\, 0 \rangle \langle \ell_1\, m_1\, \ell_2\, m_2 | L\, M \rangle$$

简化一下就是：(对于 $l_1 + l_2 + L \neq$ 奇数)

$$\int_{4\pi} Y_{\ell_1}^{m_1*} Y_{\ell_2}^{m_2*} Y_L^M \, d\Omega \propto \langle \ell_1\, m_1\, \ell_2\, m_2 | L\, M \rangle$$

3-j表示和球谐函数的关系

$$\int Y_{l_1 m_1}(\theta,\varphi) Y_{l_2 m_2}(\theta,\varphi) Y_{l_3 m_3}(\theta,\varphi) \, \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\varphi$$
$$= \sqrt{\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

35. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over every coefficient, *e.g.*, for $-8/15$ read $-\sqrt{8/15}$.

Notation:

J	J	...
M	M	...
m_1	m_2	
m_1	m_2	Coefficients
.	.	
.	.	
.	.	

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$

$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$$

$$d^\ell_{m,0} = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^m e^{-im\phi}$$

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle$$

注意顺序

$$d^J_{m',m} = (-1)^{m-m'} d^J_{m,m'} = d^J_{-m,-m'}$$

$$d^1_{0,0} = \cos\theta \qquad d^{1/2}_{1/2,1/2} = \cos\frac{\theta}{2} \qquad d^{1/2}_{1/2,-1/2} = -\sin\frac{\theta}{2}$$

$$d^1_{1,1} = \frac{1+\cos\theta}{2} \qquad d^1_{1,0} = -\frac{\sin\theta}{\sqrt{2}} \qquad d^1_{1,-1} = \frac{1-\cos\theta}{2}$$

$$d^{3/2}_{3/2,3/2} = \frac{1+\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{3/2,1/2} = -\sqrt{3}\frac{1+\cos\theta}{2}\sin\frac{\theta}{2}$$

$$d^{3/2}_{3/2,-1/2} = \sqrt{3}\frac{1-\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{3/2,-3/2} = -\frac{1-\cos\theta}{2}\sin\frac{\theta}{2}$$

$$d^{3/2}_{1/2,1/2} = \frac{3\cos\theta-1}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{1/2,-1/2} = -\frac{3\cos\theta+1}{2}\sin\frac{\theta}{2}$$

$$d^2_{2,2} = \left(\frac{1+\cos\theta}{2}\right)^2$$

$$d^2_{2,1} = -\frac{1+\cos\theta}{2}\sin\theta$$

$$d^2_{2,0} = \frac{\sqrt{6}}{4}\sin^2\theta$$

$$d^2_{2,-1} = -\frac{1-\cos\theta}{2}\sin\theta$$

$$d^2_{2,-2} = \left(\frac{1-\cos\theta}{2}\right)^2$$

$$d^2_{1,1} = \frac{1+\cos\theta}{2}(2\cos\theta-1)$$

$$d^2_{1,0} = -\sqrt{\frac{3}{2}}\sin\theta\cos\theta$$

$$d^2_{1,-1} = \frac{1-\cos\theta}{2}(2\cos\theta+1)$$

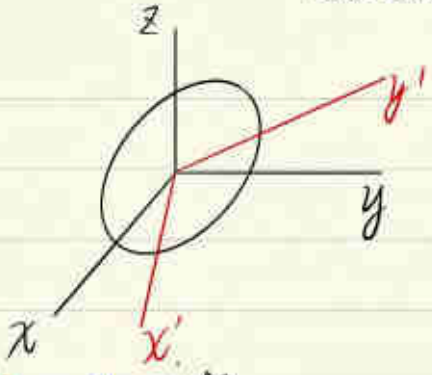
$$d^2_{0,0} = \left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

Figure 35.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

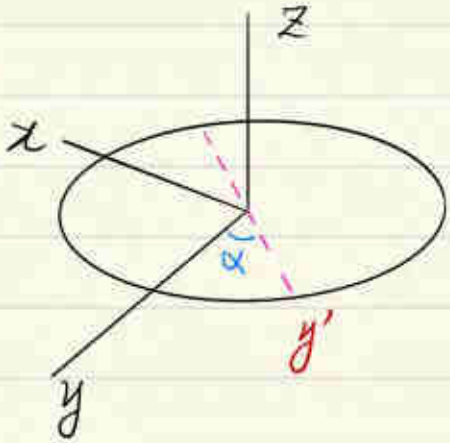
2.2 Rotation

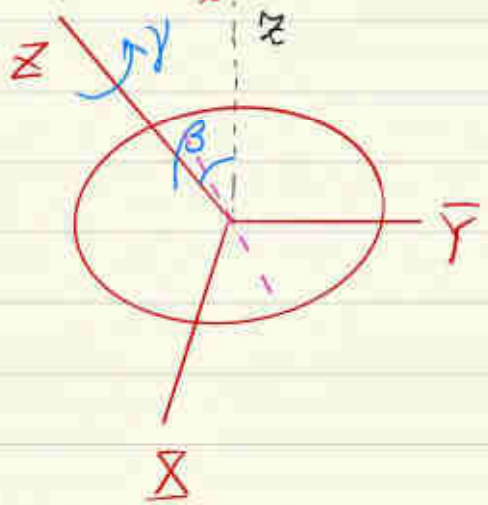
z is the quantization axis

绕z轴的转动 $|jm\rangle \to e^{-im\alpha}|jm\rangle$



三维旋转:





① 绕z转α ② 绕y'转β ③ 绕Z转γ

另外一种描述转动的办法:

绕着原来的z轴转动Gamma
绕着原来的y轴转动beta
绕着原来的z轴转动alpha

} 得到的结果和上面是一样的。(可以通过把上面第一种转动的结果用第二种方式的逆回来原位置来思考)

$$\hat{R} = e^{-i\frac{\hat{J}_z}{\hbar}\alpha} e^{-i\frac{\hat{J}_y}{\hbar}\beta} e^{-i\frac{\hat{J}_z}{\hbar}\gamma}$$

$$\Rightarrow \hat{R}|jm\rangle = \sum_{m'=-j}^{+j} |jm'\rangle\langle jm'|\hat{R}|jm\rangle$$

$$= \sum_{m'=-j}^{+j} |jm'\rangle e^{-i(m'\alpha+m\gamma)} \underbrace{\langle jm'| e^{-i\frac{J_y}{\hbar}\beta} |jm\rangle}_{\text{定义为 } d^j_{m'm}(\beta)}$$

查表即可 例如, $d^{\frac{1}{2}} = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \xrightarrow{\text{绕 } y \text{ 转 } \theta} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \xrightarrow{\text{绕 } y \text{ 转 } \frac{\pi}{2}} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

2.3

费米黄金规则(Fermi's Golden Rule)

这个工作的大部分其实是狄拉克完成的。它表达了一个能级自发跃迁的速率，亦即寿命。利用矩阵元来表示：

$$\Gamma_{i\to f} = (\frac{1}{\tau})_{E1} = \frac{2\pi}{\hbar}|\langle f|H'|i\rangle|^2\rho(E_f) \propto f_{ij}$$

其中，$\rho(E_f)$ 是态密度。f_{ij} 是跃迁强度/谐振强度(osillator strength). 它满足下面的条件(g为简并度):

$$g_i f_{ij} = g_j f_{ji}$$

而且，它还满足一个类似概率的公式：

$$\sum_j f_{ij} = 1, \quad j \neq i$$

因此，在费米规则下，我们可以得到：

$$\begin{aligned}\Gamma_{i\to f} &\propto |\langle f|H'|i\rangle|^2 \propto |\mathbf{E}\cdot\langle f|\mathbf{r}|i\rangle|^2 \\ &\propto \sum_g E_g^2|\langle l_i m_i 1g|l_f m_f\rangle|^2\end{aligned}$$

由上式，我们可以将根据 g 的取值，将跃迁分为3种：$\pi, \sigma_\pm$ 跃迁，分别对应 $g=0$ 和 $g=\pm 1$，与正常Zeeman效应相对应。（设z轴为量子轴）

对于 π 跃迁（π -transition）. 光传播的方向是在x-y平面上，但是电场沿着量子轴的方向。

对于 $\sigma_\pm$ 跃迁（$\sigma_\pm$ -transition）. 光传播的方向沿着量子轴z轴的方向，正方向为面对着光，逆时针旋转。负方向为顺时针旋转。

我们认为一个光子带一份的动量，因此，上述变换则证明了这是个单光子的跃迁。

因此，我们可以得到，E1跃迁的选择定则了（考虑LS耦合）：

1. $\Delta J = 0, \pm 1$ 因为单光子的角动量为1.
2. $\Delta S = 0$ 电子自旋不变。(假设)
3. $\Delta L = 0, \pm 1$ 初末态宇称相反。
4. $\Delta m = 0, \pm 1$ 因为g可以取0或正负1.
5. 当 $l: 0 \to 0$ 的跃迁被禁止，因为 $\langle 001g|00\rangle = 0$

注意，即便满足选择定则也不一定跃迁，在合法的CG系数中也有一些是为0的。比如：

$\langle 1010|10\rangle = 0$

2.4 Electric dipole transition $E1\ (2^a,\ a=1)$

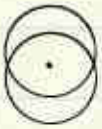
Classical: $\frac{1}{\tau} = \frac{1}{6\pi\varepsilon_0}\frac{e^2\omega^2}{mc^3}$, $\tau \sim ns$

QM: 需要一个Hamiltonian，表示电偶极与电磁场之间的耦合。

$$H' = -\vec{d}\cdot\vec{E} = e\vec{r}\cdot\vec{E} \xrightarrow{\text{平面波}} e\vec{r}\cdot\vec{E}_0 e^{i(\vec{k}\vec{r}-\omega t)}$$

开始做近似： $k = \frac{2\pi}{\lambda}$ ，而 $r \sim 0.05\,nm$ ，$\lambda \sim 500\,nm$.

所以相位里面第一项可以忽略，即认为原子某一时刻感受到的是一个均匀电场。



↕上下振动 dipole oscillation

(mono- 1

di-, bi- 2

tri- 3

quad- 4

penta- 5

deca- 10)

把Hamiltonian代入Fermi Golden Rule，得到跃迁速率：

$$A_{E1} = \left(\frac{1}{\tau}\right)_{E1} = \frac{1}{3\pi\varepsilon_0}\frac{e^2\omega^3}{\hbar c^3}\left|\langle i|\vec{r}|k\rangle\right|^2$$

$$= \left(\frac{1}{\tau}\right)_{classical}\frac{2m\omega}{\hbar}\left|\langle i|\vec{r}|k\rangle\right|^2$$

$$= -\left(\frac{1}{\tau}\right)_{classical}\cdot 3 f_{ki}$$

定义oscillator strength： f_{ki}

振子强度可以通过查表得到。

$f_{ki} < 0$. k 是上态，i 是下态. $k \to i$ 发出光子.

平衡条件： $\underbrace{g_i f_{ik}}_{\text{absorption}} = \underbrace{-g_k f_{ki}}_{\text{decay}}$

sum rule $\sum_{n\neq k} f_{kn} = 1$

$$\vec{a} = a_x\hat{x} + a_y\hat{y} + a_z\hat{z}$$

$$= -a_{+1}\hat{\varepsilon}_{-1} - a_{-1}\hat{\varepsilon}_{+1} + a_0\hat{\varepsilon}_0 \qquad \text{spherical}$$

$$\begin{cases} \hat{\varepsilon}_{+1} = -\frac{1}{\sqrt{2}}(\hat{x}+i\hat{y}) \\ \hat{\varepsilon}_0 = \hat{z} \\ \hat{\varepsilon}_{-1} = \frac{1}{\sqrt{2}}(\hat{x}-i\hat{y}) \end{cases} \qquad \begin{cases} a_{+1} = -\frac{1}{\sqrt{2}}(a_x+ia_y) \\ a_0 = a_z \\ a_{-1} = \frac{1}{\sqrt{2}}(a_x-ia_y) \end{cases} \Leftrightarrow \quad a_q = a\sqrt{\frac{4\pi}{3}}\,Y_{1q}(\theta,\varphi)$$

（即 $\vec{a} = \sum_q (-1)^q a_q \hat{\varepsilon}_{-q}$ ）

点乘： $\vec{a}\cdot\vec{b} = \sum_q (-1)^q a_q b_{-q}$

这样定义是与旋转有关的，例如对于升降算符： $[\hat{L}_+, \hat{\varepsilon}_0] = \sqrt{2}\hbar\hat{\varepsilon}_1$

Wigner- Eckart Theorem for vector

$$\langle n'j'm'|\vec{r}|njm\rangle = \sum_q (-1)^q \hat{\varepsilon}_{-q}\sqrt{\frac{4\pi}{3}}\,\underbrace{\langle n'j'\|r\|nj\rangle}_{\text{表示具体径向}}\,\underbrace{\langle j'm'1q|jm\rangle}_{\text{角向}}$$

后面1的出现，与r是一阶张量有关，即矢量。
矢量在球坐标可以用球谐函数来表示。

② $\vec{r}$ 的Parity是odd，所以必须有第三条：Parity change

① 须满足： $m = m' + q \quad (q = \pm 1)$ ，故 $\Delta M = 0, \pm 1$

② 由于 q 前面是1，为了 j'-j 构成三角形，必须有 $\Delta J = 0, \pm 1$
但是当 $j' = j = 0$ 时，不能构成 故 $0 \leftrightarrow 0$ 是禁戒的

③ 单电子情形，one electron jump， l 的奇偶即宇称奇偶，只能 $\Delta l = \pm 1$

20210330 Tuesday

$\hat{\varepsilon}_{-q}$ Tells us the polarization of light.

$$\begin{cases} \hat{\varepsilon}_{+1} = -\frac{1}{\sqrt{2}}(\hat{x}+i\hat{y}) & : \sigma^+ \\ \hat{\varepsilon}_0 = \hat{z} \\ \hat{\varepsilon}_{-1} = \frac{1}{\sqrt{2}}(\hat{x}-i\hat{y}) & : \sigma^- \end{cases}$$

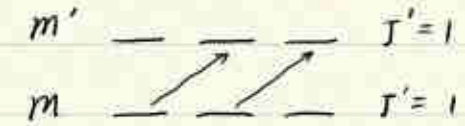
i 表示的是Pi/2的相位差，是一个圆偏振。

光的相位是很容易调控的，例如在光路中加介质。（频率是个很好的东西，在介质中，变的是波长，光速，但是不变的是频率）

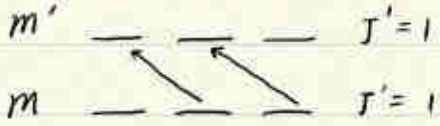
偏振片： polarizer
波片： wave plate

lambda over four wave plate 　$\frac{\lambda}{4}$ 波片

根据CG系数表，10不能到10发生跃迁。$\langle 10|1010\rangle = 0$



吸收一个σ^+光子



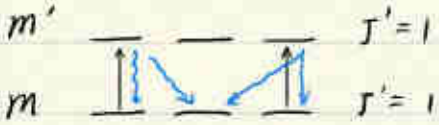
吸收一个σ^-光子

或者用球谐函数算，是的3次方。积分出来是0

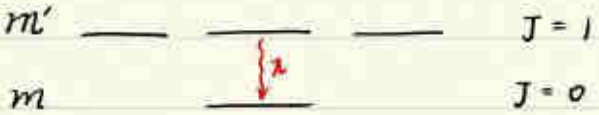
打光打上去之后，会发生自发跃迁。根据选择定则，上面的0会落到下面的1和−1。这样打sigma plus的过程，会逐渐积累在下面的+1的态。会逐渐把态输运到m最大的态。Optical Pumping

同理，这样子打sigma minus就可以把态制备到m最小的态

不会被激发的态，称为dark state。



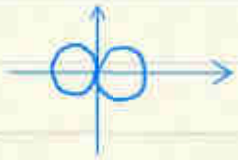
打一个π偏振的光，就会堆积到下面的0态，即dark state。

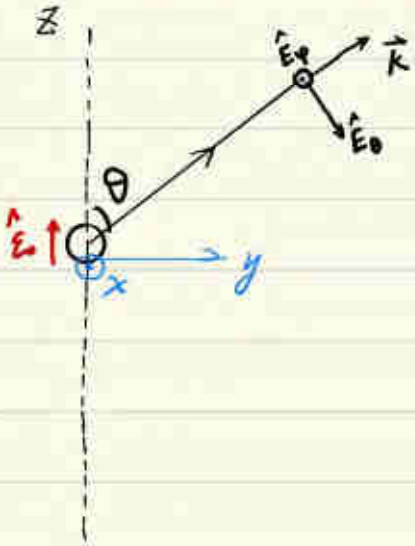


$E_\theta \propto \sin\theta$

$\text{Intensity} \to \frac{\text{Power}}{\text{Area}} \propto |E|^2 \propto \sin^2\theta$

$\text{Power} \to \frac{\text{Energy}}{\text{Time}}$



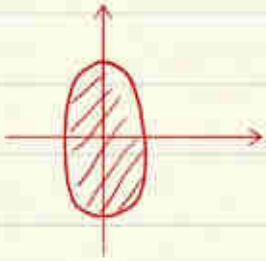


注意：虽然量子化轴本身就是随意选取的，但是，我们说一个态是态 | 10>，就已经是在确定的轴下面。要再换轴的话，相应的态会发生变化，但是最后算出来的E正比于sintheta是不会变的。

$\hat{E}_\varphi$与$\hat{x}$同向

当 $\varepsilon_+ = \frac{\hat{x} - i\hat{y}}{\sqrt{2}}$

$$I(\theta) = \left(\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{\cos\theta}{\sqrt{2}}\right)^2 = \frac{1}{2}(1+\cos^2\theta)$$



2.5 Wigner-Eckart Theorem

$\langle n' J' m' | T^L_M | n J m \rangle$ $\qquad T^L_m$ is Tensor rank L

$= \langle n' J' \| T^L \| n J \rangle \langle J' m' | L M J m \rangle \frac{1}{\sqrt{2J+1}}$

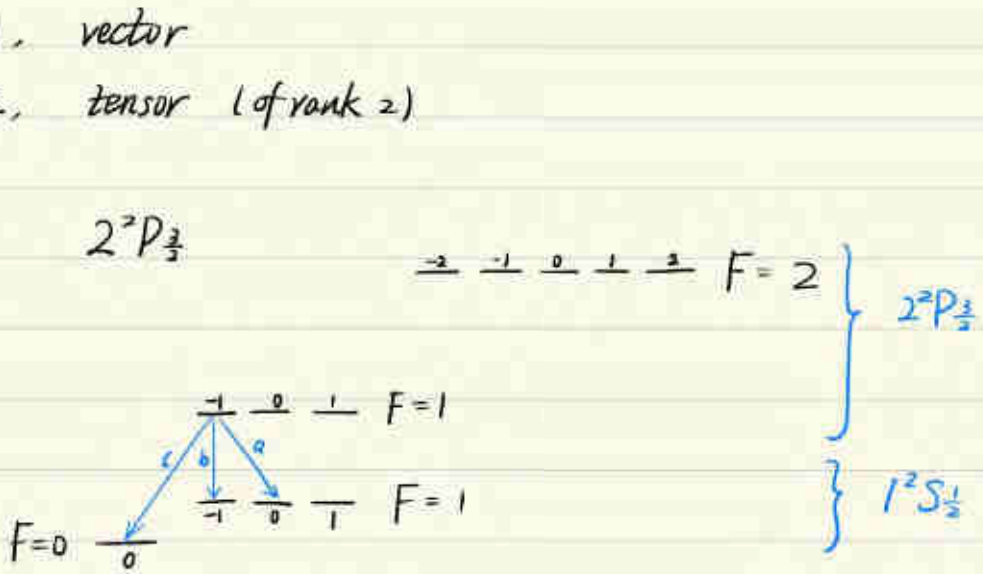
$L=0$, scalar

$L=1$, vector

$L=2$, tensor (of rank 2)

$1^2S_{\frac{1}{2}}$ $\qquad 2^2P_{\frac{3}{2}}$

$I=\frac{1}{2}$



初态 光子 末态

循环跃迁：cycling transition

ⓐ: $\langle 1\,-1 \; 1\,+1 | 1\,0 \rangle$ $\qquad -\sqrt{\frac{1}{2}}$

ⓑ: $\langle 1\,-1, 1\,0 | 1\,-1 \rangle$ $\qquad -\sqrt{\frac{1}{2}}$

F m_F $\qquad$ F m_F

(找 1×1 里面，$m_1=-1$，$m_2=1$，$M=1$，$m=0$)

$\Rightarrow B_a = B_b$

ⓒ. 上面：$J'=\frac{3}{2}$，$I=\frac{1}{2}$：

$|F=1, m_F=-1\rangle = \frac{1}{2}|-\frac{1}{2}, -\frac{1}{2}\rangle - \frac{\sqrt{3}}{2}|-\frac{3}{2}, \frac{1}{2}\rangle$

m_J m_I $\qquad$ m_J m_I

找 $\frac{3}{2}\times\frac{1}{2}$ 里面，

		$\frac{1}{2}$
$-\frac{1}{2}$	$-\frac{1}{2}$	$\boxed{\times}$
$-\frac{3}{2}$	$+\frac{1}{2}$	$\boxed{\times}$

下面：$J'=\frac{1}{2}$，$I=\frac{1}{2}$：

$\begin{cases} b: |F=1, m_F=-1\rangle = |-\frac{1}{2}, -\frac{1}{2}\rangle \\ c: |F=0, m_F=0\rangle = \frac{1}{\sqrt{2}}\left(|-\frac{1}{2}, +\frac{1}{2}\rangle - |\frac{1}{2}, -\frac{1}{2}\rangle\right) \end{cases}$

这样，Wigner-Eckart 公式的部分相同了，比较 b.c.

b: $\frac{1}{2}\langle \frac{1}{2}\,-\frac{1}{2}\;10 | \frac{3}{2}\,-\frac{1}{2}\rangle$

(E1 transition 与核自旋无关，故 m_I 不会变，只能从 跳到

$\frac{1}{2}\langle \frac{1}{2}\,-\frac{1}{2}\;10 | \frac{3}{2}\,-\frac{1}{2}\rangle = \frac{1}{2}\sqrt{\frac{2}{3}}$

J' m_J $\qquad$ J' m_J

c: $\frac{1}{2}\sqrt{\frac{1}{2}}\langle \frac{1}{2}, \frac{1}{2}, 1, -1 | \frac{3}{2}\,-\frac{1}{2}\rangle + \frac{\sqrt{3}}{2}\sqrt{\frac{1}{2}}\langle \frac{1}{2}\,-\frac{1}{2}, 1, -1 | \frac{3}{2}\,-\frac{3}{2}\rangle = \frac{1}{2}\left(\sqrt{\frac{1}{6}} + \sqrt{\frac{3}{2}}\right)$

则比例：$\frac{b}{c} = \frac{\left(\frac{1}{2}\sqrt{\frac{2}{3}}\right)^2}{\left[\frac{1}{2}\left(\sqrt{\frac{1}{6}}+\sqrt{\frac{3}{2}}\right)\right]^2} = \frac{1}{4}$

综上：$c : b : a = \frac{4}{6} : \frac{1}{6} : \frac{1}{6}$

算出来总是有理数，比例里面不会出现无理数。

Wigner进一步发现了存在在这里面的对称性。发明了6j系数。

现在：

$$\begin{matrix} J \\ I \end{matrix} > F$$

$$\begin{matrix} J' \\ I \end{matrix} > F'$$

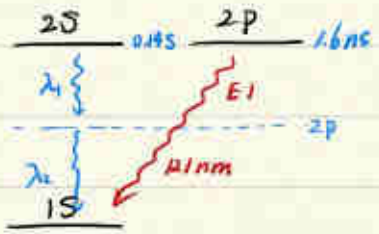
这两个之间做跃迁

然后：

$$\langle n'F'm'J'I | r_q | nFMJI \rangle$$

$$= (-1)^{J'+I-m_F'} \sqrt{(2F+1)(2F'+1)} \underbrace{\begin{Bmatrix} J' & F' & I \\ F & J & 1 \end{Bmatrix}}_{6j\text{符号}} \underbrace{\begin{pmatrix} F & 1 & F' \\ m_F & q & -m_F' \end{pmatrix}}_{3j\text{符号}} \langle n'J' \| r \| nJ \rangle$$

约化部分



2s可以通过发生双光子跃迁到达1s

事实上能级都有一定的能宽。2p能级有一定的范围，又很小的几率可以作为“中间态”。

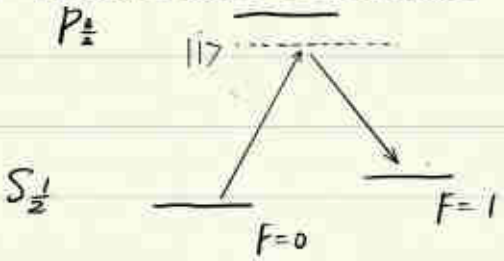
$$\frac{1}{\lambda_1}+\frac{1}{\lambda_2}=\frac{1}{121\,nm}$$

也可以激发。

最简单就是选一个242nm的激光，就可以从1s跳到2s:双光子激发

如果光是对着打的，双光子跃迁可以把一阶多普勒效应抵消掉。双光子跃迁是一个Doppler-free 过程。

另一种双光子跃迁：Raman跃迁



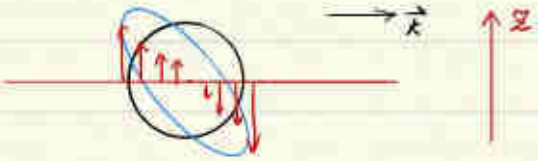
不能直接跃迁，因为没有parity change

2.6 E2 electric quadrupole transition

$$e^{i(kx-\omega t)} = e^{-i\omega t} e^{ikx} \approx e^{-i\omega t}(1 + ikx)$$

E1 E2

进一步考虑电场梯度，造成电子云的畸变



$\vec{H}' = e\vec{r}\cdot\vec{E} \propto zx \propto Y_{2,\pm 1}$ tensor of rank 2

跃迁与有关：$\langle JM | Y_{2,m} | J'M' \rangle$

$\propto \langle JM | 2m\, J'M' \rangle$

Electric quadrupole

$\Delta J = 0, \pm 1, \pm 2$
$(0 \not\leftrightarrow 0;\ \frac{1}{2} \not\leftrightarrow \frac{1}{2};\ 0 \not\leftrightarrow 1)$ 三角形定则的要求

$\Delta M = 0, \pm 1, \pm 2$

No parity change $Y_{2,m}$ 的宇称是偶的

One or no electron jump
$\Delta I = 0, \pm 2$ （同样是由于宇称的原因）

$\Delta S = 0$ 该跃迁与自旋无关

$\Delta L = 0, \pm 1, \pm 2$
$(0 \not\leftrightarrow 0;\ 0 \not\leftrightarrow 1)$

矩阵相差kx，所以跃迁速率相差(kx)^2的量级

$$\frac{E2\ rate}{E1\ rate} \sim (ka_0)^2 \sim \left(\frac{2\pi}{\lambda}a_0\right)^2 \sim 10^{-6}$$

E1的寿命在ns量级，而E2的寿命在ms量级

E2跃迁慢，频宽很窄。而E1的自然线宽很宽，大概是MHz。 $\frac{\Delta f}{f}$

所以做原子钟，可以用E2跃迁

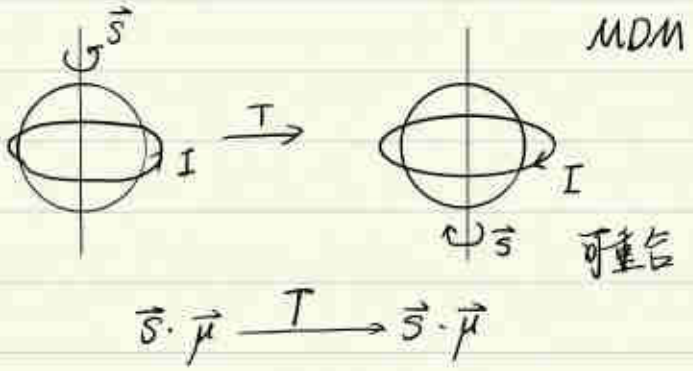
（还有用^{229}Th 的，nuclear clock）

注意在电四极跃迁中，需要考虑原子的大小。发出的过程仍然是单光子过程，只不过携带走2的角动量。（例如考虑上光子的轨道角动量）

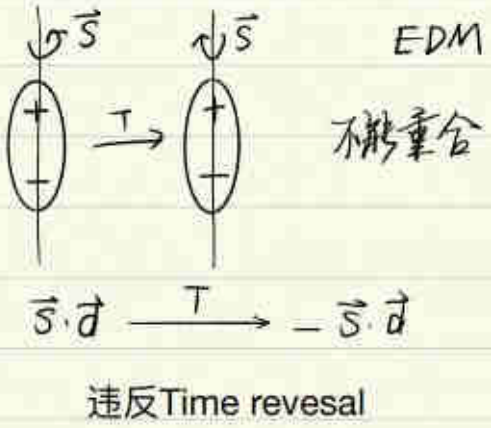
Nuclear moment

	B	E
monopole	?	e
dipole	$\vec{M}$	?

对于核来说，只要有自旋，就有磁偶极矩。



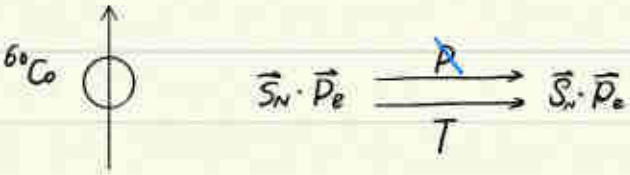
Electric dipole moment



违反Time revesal

axial vector 轴矢量

验证宇称不守恒：破坏空间反演对称性　　P odd，T even



然后Laudau说，P在这个实验中被破坏了，但是可以通过：

left particle $\Longleftrightarrow$ right $\overline{\text{particle}}$ → 反粒子

在物理定律里面被同样对待，称为CP守恒

然后被验证其实...也可以被破坏

于是有了CPT对称性，到目前为止没有被破坏，并且被量子场论所证实。
是一个好的对称性。自然界是区分左右的。

所以时间不是一个好的对称性。所以我们认为，电偶极矩应该存在。

Nuclear moment

	B	E
monopole	?	e
dipole	$\vec{M}$	? ≈ 0
quadrupole	0	Q

→ 不违反任何对称性，是P even，T even的。

自旋等于0的原子，核等，一定没有EDM和MDM

$$\langle jm|\vec{\mu}|jm\rangle \propto \langle \| \| \rangle \langle jm|1q\,jm\rangle \quad , j\neq 0$$

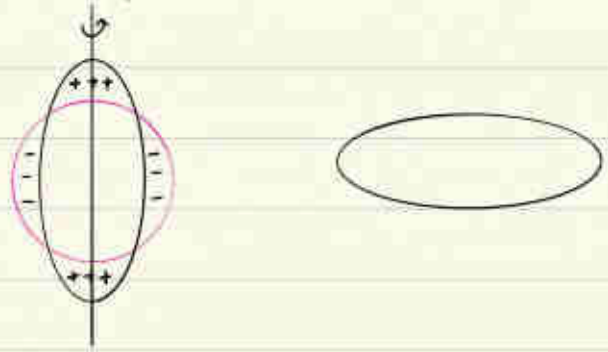
电四极矩也有角动量的要求：

$$\langle jm|Q|jm\rangle \propto \langle jm|2q\,jm\rangle \quad , j\neq 0, \frac{1}{2}$$

所以自旋是1/2的粒子，例如电子质子等，都没有电四极矩

电四极矩的形状

橄榄形 prolate　　oblate



$aY_{00} + bY_{20}$

只有 Y_{20}，是轴对称的，没有 Y_{21}.

$3z^2 - r^2 = 2z^2 - x^2 - y^2$

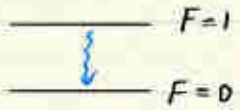
2.7 M2 (magnetic dipole transition)

与磁场的耦合

$$\left(\frac{1}{\tau}\right)_{M1} = \frac{\mu_0 \omega^3}{2\pi\hbar c^3} |\langle i|\vec{\mu}|f\rangle|^2$$

$$\frac{\left(\frac{1}{\tau}\right)_{M1}}{\left(\frac{1}{\tau}\right)_{E1}} = \frac{1}{c^2}\frac{\mu^2}{(er)^2} \sim \left(\frac{1}{2}Z\alpha\right)^2 \sim 10^{-5}$$

$^2S_{\frac{1}{2}}$



1420 MHz，21cm 波

TABLE 7.1.

Selection rules for single photon transitions in atomic spectra

Rule	Electric dipole	Magnetic dipole	Electric quadrupole
1.	$\Delta J = 0, \pm 1$ $(0 \not\leftrightarrow 0)$	$\Delta J = 0, \pm 1$ $(0 \not\leftrightarrow 0)$	$\Delta J = 0, \pm 1, \pm 2$ $(0 \not\leftrightarrow 0;\ \frac{1}{2} \not\leftrightarrow \frac{1}{2};\ 0 \not\leftrightarrow 1)$
2.	$\Delta M = 0, \pm 1$	$\Delta M = 0, \pm 1$	$\Delta M = 0, \pm 1, \pm 2$
3.	Parity change	No parity change 严是轴矢量	No parity change
4.	One electron jump $\Delta l = \pm 1$	No electron jump $\Delta l = 0, \Delta n = 0$	One or no electron jump $\Delta l = 0, \pm 2$
5.	$\Delta S = 0$	$\Delta S = 0$	$\Delta S = 0$
6.	$\Delta L = 0, \pm 1$ $(0 \not\leftrightarrow 0)$	$\Delta L = 0$	$\Delta L = 0, \pm 1, \pm 2$ $(0 \not\leftrightarrow 0;\ 0 \not\leftrightarrow 1)$

进行耦合之后，原来这些角动量都不是exact quantum number，会与其他的角动量混一点儿。即指态会发生重组，原来不是好量子数了。

Chapter3 Other Effect

3.1 Zeeman 效应

弱场情况，（$\mu_B B < A$）

已知，电子的磁矩由轨道磁矩和自旋磁矩组成：

$$\mu = -g_L \mu_B L - g_S \mu_B S$$

但是，在弱场时，我们可以用J表达。因为 $J = L + S$，而 $g_L \neq g_S$，所以显然，μ_J 与 $\mu_L + \mu_S$ 的方向不同。但是，由图可知，图中的圆为运动轨迹。我们可以看到，μ 是实际的磁矩，它的运动的平均值就是 μ_J. 所以当旋转很快速的时候，可以用它的平均值来代替。

因此，我们让它对于J求平均值，然后让它约为它的平均值。最后得到了 g_J 的表达式和平均的磁矩的表达式。

$$\mu_J \approx \langle \mu_J \rangle = \frac{\langle \mu \cdot J \rangle}{\langle J^2 \rangle} J = -g_J \mu_B J$$

所以g因子的表达式：（这里，$g_J = 1$，$g_S = 2$）

$$\begin{aligned} g_J &= \frac{g_L \langle L \cdot J \rangle + g_S \langle S \cdot J \rangle}{\langle J^2 \rangle} \\ &= \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)} \end{aligned}$$

由于最开始的近似，我们认为这种磁场的影响不包括核磁矩的影响，但是，却包括超精细结构的影响（即，我们认为本征态为 $|FM_F\rangle$）。因此，我们将利用微扰理论去处理弱磁场的作用。（同时，微扰理论也意味着，这里的弱磁场表达的是 $\mu_B B < A$）。因此，仿照上面的做法，我们定义新的g因子和磁矩。

$$\begin{aligned} \mu_F \approx \langle \mu_F \rangle &= \frac{\langle \mu_J \cdot F \rangle}{\langle F^2 \rangle} F = -g_J \mu_B \frac{\langle J \cdot F \rangle}{\langle F^2 \rangle} F \\ \langle J \cdot F \rangle &= \langle F^2 + J^2 - I^2 \rangle / 2 \\ g_F &= g_J \frac{f(f+1) + f(f+1) - i(i+1)}{2f(f+1)} \end{aligned}$$

在这样的定义下面：

$$\begin{aligned} H' &= -\mu_F \cdot B = g_F \mu_B F \cdot B = g_F \mu_B B F_z \\ E &= \langle H' \rangle = g_F \mu_B B M_F \end{aligned}$$

因此，我们得到了，在弱磁场下，原先的一条线会变为（2F+1）条线，每个F的投影都对应一条线。而且正比于磁场强度。

可计算，与实验符合

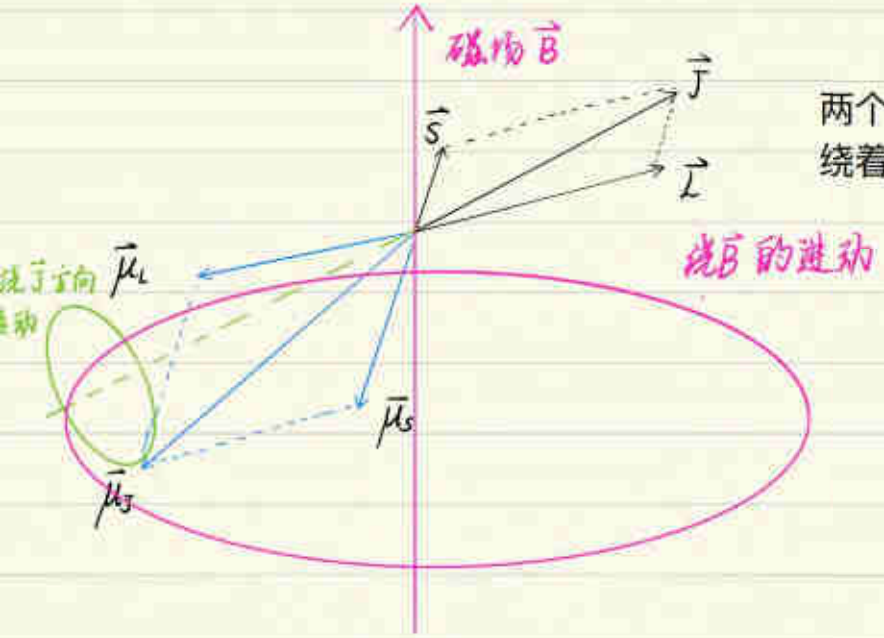
磁偶极矩 $\begin{cases} \vec{\mu}_L = -g_L \mu_B \dfrac{\vec{L}}{\hbar} & g_L = 1 \\ \vec{\mu}_S = -g_S \mu_B \dfrac{\vec{S}}{\hbar} & g_S \approx 2 \\ \vec{\mu}_N = +g_p \mu_N \dfrac{\vec{L}}{\hbar} & g_p = 5.6 \cdots \end{cases}$ $\mu_B = \dfrac{e\hbar}{2m_e}$ Bohr Magneton

质子

$\mu_N = \dfrac{e\hbar}{2m_N}$ Nuclear magneton

中子 $g_n = -3.8 \cdots$ 目前无法理论精确计算，只能实验测

因为质子和中子有结构，不能看成是点粒子，因此Dirac方程不能描述质子和中子，因此用Dirac方程不能预测质子中子的g。（而到目前为止都认为电子是点状的，无结构。）对电子的预测，用量子电动力学就可以。而质子和中子需要用量子色动力学描述，并且还没有发展好，不能很精确预测。



两个角动量的相互作用，产生力，导致了mu_j绕着J的转动。

① $\vec{\mu}_J$ 进动的频率可以用精细结构中LS耦合的能量计算，能量大概是 $0.1\ cm^{-1}$
$\sim 3\times 10^{9}\ Hz$

② $\mu_B = 9\times 10^{-12}\ J/T$ 对应 $1.4\ MHz/G$
当 $B = 100G$，是 $10^{8}\ Hz$

所以如果要用下面的理论，即忽略mu_j绕着J的进动，需要频率①远高于频率②

weak-field approx. 弱场进似

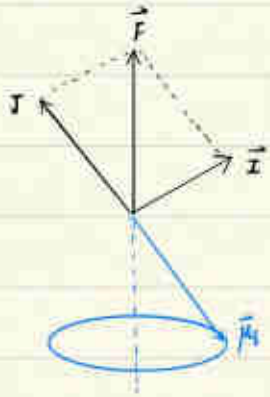
$$\begin{cases} H_{Zeeman} = -\dfrac{(\vec{\mu}_L+\vec{\mu}_S)\cdot\vec{J}}{|\vec{J}|}\left(\dfrac{\vec{J}}{|\vec{J}|}\cdot\vec{B}\right) \\ \text{有效 } \vec{\mu}_J = -g_J \mu_B \dfrac{\vec{J}}{\hbar} \end{cases}$$

弱磁场下的Zeeman位移

并利用 $\vec{J}-\vec{L}=\vec{S} \Rightarrow \vec{J}^2+\vec{L}^2-2\vec{J}\cdot\vec{L}=\vec{S}^2$

$$\Rightarrow \quad g_J = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)}$$

再与原子核耦合，并注意到原子核的 μ_N 远小于电子的 μ_B，所以就不考虑原子核的磁矩的影响，在考虑进动的时候仍然只考虑mu_j的影响。



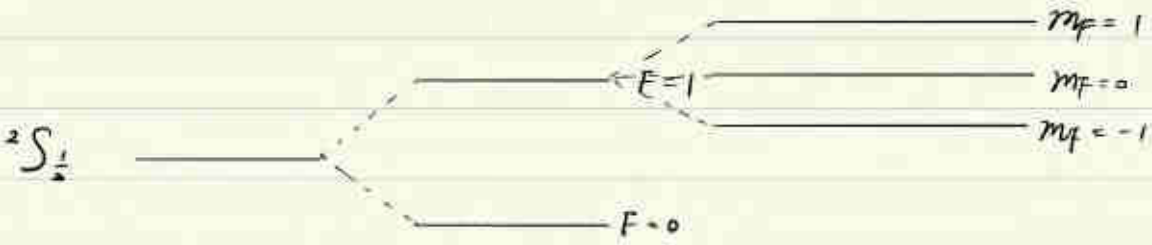
$$g_F = \frac{F(F+1)+J(J+1)-I(I+1)}{2F(F+1)}\, g_J$$

先绕$\vec{F}$转，再绕外场$\vec{B}$转。

这里mu_j仍然与J平行，是已经采取了上面的近似。

并且由于超精细结构的能量分裂更小，在做这个近似的时候，对弱场的要求更高。

对氢原子基态：



$g_F = \frac{1}{2} g_J = 1, \quad g_J = 2$ (weak field)

$$\vec{H} = -\vec{\mu}\cdot\vec{B}$$
$$= -\left(-g_F \mu_B \frac{\vec{F}}{\hbar}\right)\cdot \vec{B}$$
$$= g_F \mu_B m_F B$$

3.2 Multipole Expansion

极距的多级展开（Multipole expansion）

电多极距

原子核是具有电荷和磁矩。如何理解原子核呢？我们从电场和磁场的单极距，偶极矩，四极矩等进行考察：将电势展开：

$$V(\vec{r}) = \int \frac{1}{4\pi\epsilon_0} \frac{\rho(\vec{r_N})}{|\vec{r} - \vec{r_N}|} d^3 r_N$$

由数理方程知道，勒让德多项式(Legendre polynomial) 的母函数为：（ θ 为两个 r 之间的夹角）

$$\frac{1}{|\vec{r} - \vec{r_N}|} = \sum_k \frac{r^k}{r_N^{k+1}} P_k(\cos\theta)$$

而且，勒让德函数与球谐函数具有关系：

$$P_k(\cos\theta) = \frac{4\pi}{2k+1} \sum_{q=-k}^{k} (-1)^q Y_{k,-q}(\theta_N, \phi_N) Y_{k,q}(\theta, \phi)$$

我们不妨分级去展开。当 $k=0$ 时，我们考虑的是单极距monopole. 此时， $Y_{0,0} = \sqrt{1/4\pi}$ 因此， $P_0 = 1$ 。同理， $k=1$ 时， $P_1(\cos\theta) = \cos\theta$ 。等等，总结为下：取 $1/4\pi\epsilon_0 = 1$

$$\begin{aligned}
&k=0, \quad P_0(\cos\theta) = 1, && V^{(0)}(r) = \frac{\int \rho}{r} \\
&k=1, \quad P_1(\cos\theta) = \cos\theta, && V^{(1)}(r) = \frac{\int \rho r_N \cos\theta}{r^2} = \frac{\vec{p}\cdot\hat{r}}{r^2} \\
&k=2, \quad P_2(\cos\theta) = \frac{1}{2}(3\cos^3\theta - 1), && V^{(2)}(r) = \frac{\int \rho r_N^2 (3\cos^3\theta - 1)/2}{r^3} = \frac{\hat{r}^T Q \hat{r}}{r^3}
\end{aligned}$$

在上式中，我们分别定义了电偶极矩和电四极矩：

$$\begin{aligned}
\vec{p} \quad &= \int \rho \vec{r}_N \, d^3 r_N \\
Q_{ij} \quad &= \int \frac{\rho}{2} (3 r_N^i r_N^j - |r_N|^2 \delta_{ij}) \, d^3 r_N, \qquad i,j = x,y,z
\end{aligned}$$

如果我们需要的是电场，我们可以利用 $E = -\nabla V$ 得到。我们可以计算得到：

$$\begin{aligned}
&\text{monopole:} && E = \frac{e}{r^2} \\
&\text{dipole:} && E = \frac{p\cdot\hat{r}}{r^2} \\
&\text{quadrupole:} && E = \frac{\hat{r}^T Q \hat{r}}{r^3}
\end{aligned}$$

3.3 超精细结构：磁偶极矩和电四极矩的影响

先算磁偶极矩的影响：

$V \sim \frac{1}{r}$, mono – mono interaction

$V \sim \frac{1}{r^2}$, mono- dipole interaction

$V \sim \frac{1}{r^3}$, dipole - dipole interaction

$$\hat{H} = \frac{\mu_0}{4\pi}\frac{1}{r^3}\left[\vec{\mu}_e\cdot\vec{\mu}_N - \frac{3(\vec{\mu}_e\cdot\vec{r})(\vec{\mu}_N\cdot\vec{r})}{r^2} - 4\pi\delta(\vec{r})\, r^3\, \vec{\mu}_e\cdot\vec{\mu}_N\right]$$

Contact potential (Drive from $\nabla^2(\frac{1}{r}) = -4\pi\delta(r)$)

(Recall that , Darwin term in relativity is also Contact potential,
which will influence the energy of some special state.)

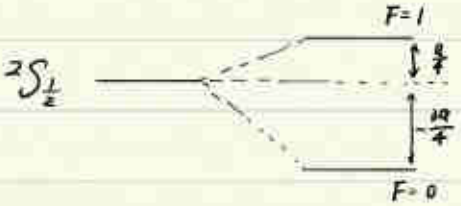
s-orbit
非 s-orbit

简化 $\Rightarrow \begin{cases} \hat{H} = a\vec{I}\cdot\vec{S} \\ \hat{H} = a_J\vec{I}\cdot\vec{J} \end{cases}$

例子： Hyperfine structure in the ground state of H

$(\vec{F} = \vec{I} + \vec{S})$

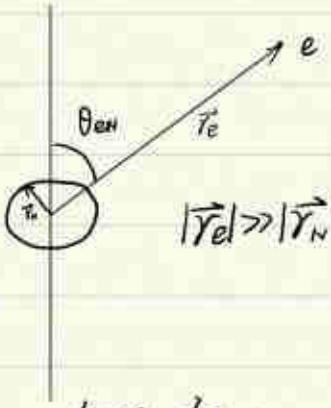
$$E_{hfs} = \frac{a}{2}\left[F(F+1) - I(I+1) - S(S+1)\right]$$



超精细结构两个不变： $\begin{cases} \text{Number of states} \\ \text{Center of "gravity" 这个可以这样解释：哈密顿量对全空间积分为0} \end{cases}$

这里 $a \sim \frac{\mu_e \mu_N}{a_0^3}$

超精细结构：电四极矩的影响：电子和核的四极矩之间的相互作用



$$E = -\frac{1}{4\pi\varepsilon_0}\int \frac{\rho(\vec{r}_e)\rho(\vec{r}_N)}{|\vec{r}_e-\vec{r}_N|}\,dr_e\,dr_N$$

$|\vec{r}_e| \gg |\vec{r}_N|$

利用级数 $\frac{1}{|\vec{r}_e-\vec{r}_N|} = \sum_k \frac{r_N^k}{r_e^{k+1}} P_k(\cos\theta_{eN})$ 做近似

$$P_k(\cos\theta_{eN}) = \frac{4\pi}{2k+1}\sum_{q=-k}^{+k}(-1)^q Y_{kq}(\theta_N,\varphi_N)\,Y_{k-q}(\theta_e,\varphi_e)$$

（$\vec{a}\cdot\vec{b} = \sum_q (-1)^q a_q b_{-q}$，球坐标中二点乘）

$K=0$ term $\quad \frac{1}{|\vec{r}_e-\vec{r}_N|} \approx \frac{1}{r_e}$，库伦相互作用

$K=1$ term 核至少有一个旋转对称轴，因此phi_N不用考虑，对应的球谐函数只要q=0的一项。

$$\frac{r_N}{r_e}P_1(\cos\theta_{eN}) = \frac{r_N}{r_e}\frac{4\pi}{3}Y_{10}(\theta_N)Y_{10}(\theta_e)$$

其他的项，积分会变成0。

z，对应核二dipole与电子云的dipole二耦合

$K=3$：
$$\frac{r_N^2}{r_e^3}\frac{4\pi}{5}Y_{20}(\theta_N)Y_{20}(\theta_e)$$
$$= \left(r_N^2 Y_{20}(\theta_N)\right)\left(\frac{1}{r_e^3}Y_{20}(\theta_e)\right)\frac{4\pi}{5}$$
$$\propto \underbrace{(3z_N^2 - r_N^2)}_{\text{核}}\left(\frac{1}{r_e^3}\frac{3\cos^2\theta_e-1}{2}\right)$$

Nuclear quadrupole moment

查表的话，一般是这种形式：

$$Q = \langle I, m_I = I \,|\, \sum_i (3z_i^2 - r_i^2) \,|\, I, m_I = I \rangle$$

质子的电四极矩等于0。（因为质子自旋1/2，不应该有电四极矩）

$$\langle \tfrac{1}{2},\tfrac{1}{2} | T_K^2 | \tfrac{1}{2},\tfrac{1}{2}\rangle = 0$$

tensor of rank 2

（但是 ^2H，$I=1$，有电四极矩，说明原子核内部力并不沿连线方向

$Q(^2H) \sim 0.3\times10^{-30}\,m^2 = 0.003$ barn

1 barn $= 10^{-28}\,m^2$ 与核对中子的吸收截面有关）

（ $Q(^{133}Cs) = -0.003$ barn，负的是核在z方向比较扁 ）

电四极矩和电场相互作用的Hamiltonian： $\hat{H} = eQ\frac{dE}{dz}$

这样，电四极矩对超精细结构的贡献：

$$E_{hfs} = A_J\,\tfrac{1}{2}\left[F(F+1) - I(I+1) - J(J+1)\right] + \frac{B}{8I(2I-1)J(2J-1)}\left[3K(K+1) - 4I(I+1)J(J+1)\right]$$

在有超精细结构下的Zeeman位移，当量级近似相同时一起算。

$^2S_{\frac{1}{2}}$ $\quad |I\ m_I\ S\ m_s\rangle$

	++	+−	−+	−−
++	$\mu_B B + \frac{a}{4}$	0	0	$\cancel{0 + \frac{a}{4} - \frac{a}{4}}$
+−	0	$-\mu_B B - \frac{a}{4}$	$0 + \frac{a}{4} + \frac{a}{4}$	0
−+	0	$0 + \frac{a}{4} + \frac{a}{4}$	$-\mu_B B - \frac{a}{4}$	0
−−	$\cancel{0 + \frac{a}{4} - \frac{a}{4}}$	0	0	$-\mu_B B + \frac{a}{4}$

仍然是本征态

其中 $\frac{a}{4}$ 为了

Example 6.3 *The Zeeman effect on the hyperfine structure of hydro*
for all field strengths

Figure 6.10 shows the energy levels for all field strengths. The Zee
energies of the $M = \pm 1$ states are $\pm\mu_B B$ for all fields because t
wavefunctions are not mixed ($g_F = 1$ from eqs 6.30). The M_F
states have no first-order shift but the magnetic field mixes these
states in the $F = 0$ and 1 hyperfine levels; the matrix element betw
them is

$$\langle F = 1, M_F = 0|\boldsymbol{\mu}\cdot\mathbf{B}|F = 0, M_F = 0\rangle = \zeta\mu_B B.$$

Such (off-diagonal) matrix elements can be evaluated by angular mom
tum theory, but in this simple case we can get by without using Cleb
Gordan coefficients (leaving ζ as an undetermined constant for the t
being). The Hamiltonian for the two-level system is

$$H = \begin{pmatrix} A/2 & \zeta\mu_B B \\ \zeta\mu_B B & -A/2 \end{pmatrix}. \qquad (6$$

太小了，忽略

$$E_{Zeeman} = 2\mu_B B m_s + 2\mu_N B m_I$$

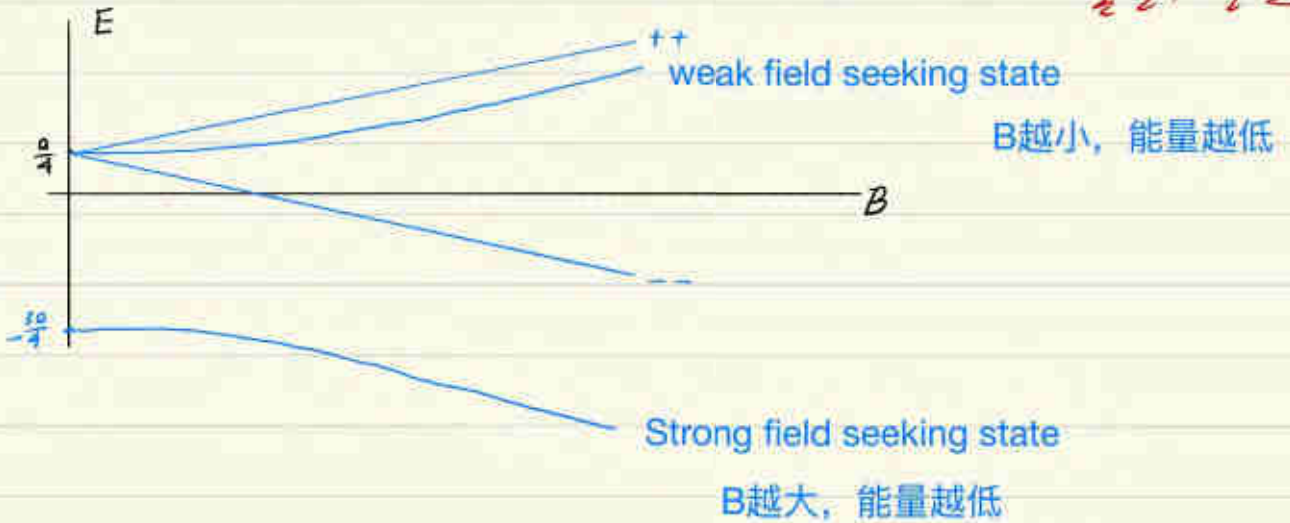
超精细结构 $\quad \hat{H} = a\vec{I}\cdot\vec{S} = \frac{a}{4}\left(\sigma_x^I\sigma_x^S + \sigma_x^I\sigma_x^S + \sigma_z^I\sigma_z^S\right)$

在非耦合表象，所以展开成这样样子算（等价于升降算符）。如果是耦合表象，就用常用的用角动量那堆平方算。

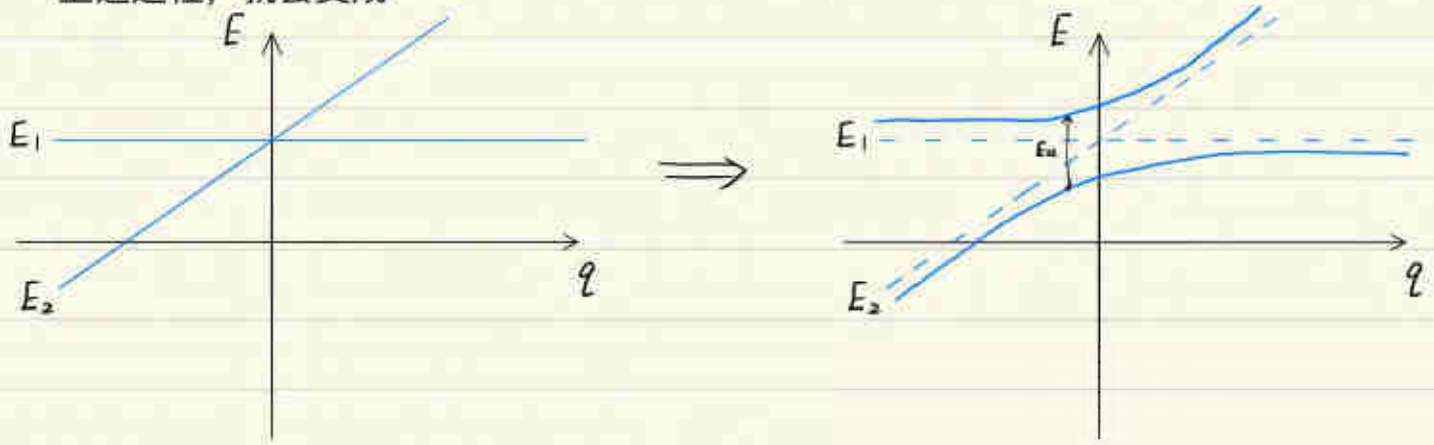
对角化， $\quad E = -\frac{a}{4} \pm \sqrt{\left(\frac{a}{2}\right)^2 + (\mu_B B)^2}$

没考虑电四极矩？

是 $\frac{a}{2}, -\frac{a}{2}$ 还是 $\frac{a}{4}, -\frac{3a}{4}$



根据矩阵的性质，如果本来对角元相同（具有相同的“能量”），但是不同态之间有耦合，即非对角项为0，那么在进行对角化之后，能量会分开。如果还有一个其他的参数q，在q=0时是上述过程，就会变成：



Adiabatic Transfer $\quad$ 条件： $\left|\frac{dE}{dt}\right| \ll \frac{E_{12}^2}{\hbar}$

Landau-Zener Transition: $P = e^{-2\pi\Gamma}$, $\Gamma = \dfrac{(E_{12}^{min}/2)^2}{\hbar\left|\frac{dq}{dt}\frac{\partial E_{12}}{\partial q}\right|}$

3.5 Stark effect

$$\hat{H}' = e\vec{r}\cdot\vec{E}$$

$$\Delta E_{stark} = e\ \langle jm|\vec{r}|jm\rangle\cdot\vec{E} = 0$$

Parity odd，和逆相同 Parity，故是0

（对比，Zeeman效应中： $\hat{H}' = -\vec{\mu}\cdot\vec{B}$，

$\vec{\mu} \propto \vec{L} + 2\vec{S}$ ，axial-vector 轴矢量都是Parity-odd

能量变化为0，但是态会发生重组。使用一阶微扰论：

$$|s'\rangle = |s\rangle + \frac{\langle p|H'|s\rangle}{E_s - E_p}$$

$$|p'\rangle = |p\rangle + \frac{\langle s|H'|p\rangle}{E_p - E_s}$$

至于哪几个态发生耦合，与所加电场方向有关。

二阶Stark Shift

$$s: \quad \Delta E^{(2)}_{stark} = \frac{|\langle s|H'|p\rangle|^2}{E_s - E_p}$$

$$p: \quad \Delta E^{(2)}_{stark} = \frac{|\langle s|H'|p\rangle|^2}{E_p - E_s}$$

（高的变高，低的变低，和刚才矩阵分析一样。）

再对比Zeeman效应，它有一阶项，是一阶效应： $Zeeman \propto m_l$ ，

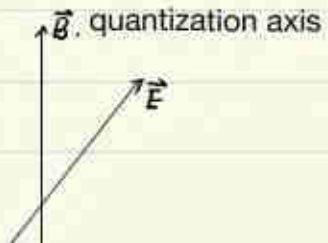
$m_l=-1$ $m_l=0$ $m_l=1$

Stark效应是2阶效应，能级的分裂是对称的： $Stark \propto m_l^2$

$$\Delta E_{stark} = -\frac{1}{2}\alpha_0\mathcal{E}^2 - \frac{1}{2}\alpha_2\mathcal{E}^2\,\frac{3\cos^2\theta - 1}{2}\,\frac{3m_F^2 - F(F+1)}{F(2F-1)}$$

α_0 Scalar polarizability

α_2 Tensor polarizability

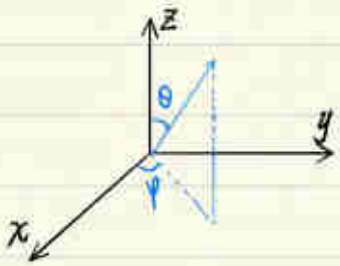


Chapter 4 Two-Level System

4.1 Spin 1/2

$|\uparrow\rangle \quad \begin{pmatrix}1\\0\end{pmatrix}$ $\qquad \sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix}, \ \sigma_y = \begin{pmatrix}0&-i\\i&0\end{pmatrix}, \ \sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$

Two-Level system $\quad |\downarrow\rangle \quad \begin{pmatrix}0\\1\end{pmatrix}$



$$\hat{\sigma} = \cos\theta\,\hat{\sigma}_z + \sin\theta\cos\varphi\,\hat{\sigma}_x + \sin\theta\sin\varphi\,\hat{\sigma}_y$$
$$= \begin{pmatrix}\cos\theta & \sin\theta\, e^{-i\varphi}\\ \sin\theta\, e^{i\varphi} & -\cos\theta\end{pmatrix}$$

$$|\psi\rangle_{op} = \begin{pmatrix}\cos\frac{\theta}{2}\, e^{-i\varphi/2}\\ \sin\frac{\theta}{2}\, e^{i\varphi/2}\end{pmatrix}$$

加入静磁场: $\quad \hat{H} = -\vec{\mu}\cdot\vec{B} = \mu_B B\,\sigma_z$

$+\mu B$ ———— $|\uparrow\rangle$

Spin up and spin down 是能量本征态

如果初始是任意态: $\quad i\hbar\partial_t\psi = \hat{H}\psi$

$-\mu B$ ———— $|\downarrow\rangle$

$$\Rightarrow \psi(t) = \begin{pmatrix}\cos\frac{\theta}{2}\, e^{-i\frac{\varphi}{2}}\, e^{-i\frac{\mu_B B}{\hbar}t}\\ \sin\frac{\theta}{2}\, e^{i\frac{\varphi}{2}}\, e^{i\frac{\mu_B B}{\hbar}t}\end{pmatrix}$$

θ constant, $\quad \varphi \to \varphi_0 + \underbrace{\frac{2\mu_B B}{\hbar}}\, t$

$\hookrightarrow$ Larmor Frequency $\quad \Omega_L = \frac{E_1 - E_2}{\hbar} = \frac{2\mu_B B}{\hbar}$

注意进动频率和倾斜角theta无关。薛定谔方程只跟波函数的一次方有关，没有高阶现象

David Wineland曾经来过肥科。

Spin $\frac{1}{2}$ $\ (\theta, \varphi) \longleftrightarrow$ 3D-vector (θ, φ) $\qquad$ Special Orthogonal 3, SO(3)

SU(2) $\quad$ 振幅 $\quad$ 相位 $\qquad$ 方向

左边这个群里面的元素比右边群的元素多一倍，来源于左边旋转2pi会改变相位

$$|\psi\rangle_{op} = \begin{pmatrix}\cos\frac{\theta}{2}\, e^{-i\varphi/2}\\ \sin\frac{\theta}{2}\, e^{i\varphi/2}\end{pmatrix} = \begin{pmatrix}a\\b\end{pmatrix} = a|\uparrow\rangle + b|\downarrow\rangle$$

$\vec{R} = (R_x, R_y, R_z)$

① $R_z = \cos\theta = \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} = |a|^2 - |b|^2 = 1 - 2|b|^2$

在z方向的投影，代表了两个态之间population的差距。

跃迁: $\quad t=0, \ |a(0)|^2 = 1, \ |b(0)|^2 = 0$

$$Prob = |b|^2 = \frac{1 - R_z}{2}$$

② $R_x = \sin\theta\cos\varphi = 2\,Re(a^* b) \sim \sin(\Omega_L t)$

③ $R_y = \sin\theta\sin\varphi = 2\,Im(a b^*)$

4.2 进动

经典力学的进动

力矩 Torq $\quad \vec{\mu}\times\vec{B} = \vec{\Omega}_L\times\vec{S} = \frac{d\vec{S}}{dt}$

$\vec{\mu} = r\vec{S}$ 原子的磁偶极矩沿着自旋方向

$\Omega_L = -\gamma B \quad \left(= \frac{2\mu_0 B}{\hbar} \Rightarrow \gamma = -\frac{2\mu_0}{\hbar}\right)$

γ 磁旋比 gyromagnetic ratio

electron : $-2\pi \cdot 2.8$ MHz / Gauss

proton : $+2\pi \cdot 4.2$ KHz / Gauss

已经有了一个强磁场，如果只加一个横向的小的静磁场，那么朝上转不下来，只会围着一个稍微有一点儿偏的方向做进动。所以不能用静磁场，而是用一个跟随其Larmor频率一起运动的转动的磁场。

用两对垂直的亥姆霍兹线圈，并使他们有pi/2的相位差。

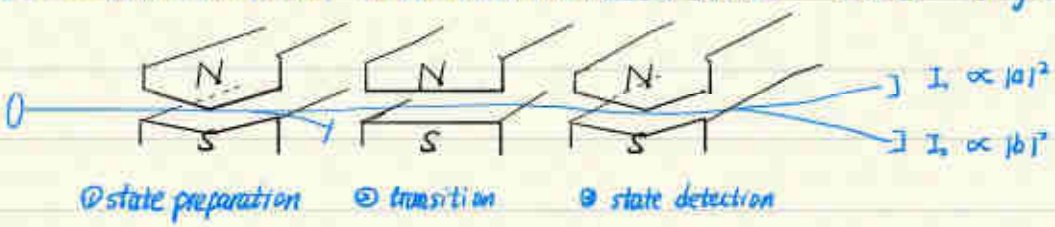
$$\begin{cases} \vec{B}_+ = B_T(\cos\omega t\,\hat{x} + \sin\omega t\,\hat{y}) \\ \vec{B}_- = B_T(\cos\omega t\,\hat{x} - \sin\omega t\,\hat{y}) \end{cases}$$

后来，只用一个线圈，并且考虑到线偏振是两个方向不同的圆偏振的叠加。

$$B_T\hat{x}\cos\omega t = \frac{1}{2}(\vec{B}_+ + \vec{B}_-)$$

利用 Rotating wave approximation, 把频率相差的远的几乎不起作用

事实上有微弱的效应，在特别精密的测量中有用： Bloch - Siegert shift



$\frac{I_1 - I_2}{I_1 + I_2} = R_z$

上面装置都横过来看

4.3 Bloch Equation

Larmor : $\Omega_L = -\gamma B$

Rotating field: ω, B_T

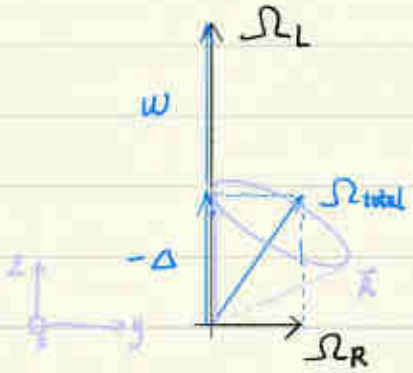
Rabi Oscillation: $\Omega_R = -\gamma B_T$

Detuning: $\Delta = \omega - \Omega_L$ $\begin{cases} \Delta > 0, \text{ blue detuning} \\ \Delta < 0, \text{ Red detuning} \end{cases}$

$\Delta = 0$, $\omega = \Omega_L$

$t_{x\text{-pulse}} = \frac{\pi}{\Omega_R}$

下面就从一个更加general的角度讲，不提磁场，而图像只有一个二能级系统，以及上面的一堆频率



转换成一个以omega运动的旋转参考系

$$-\frac{d\vec{R}}{dt} = (-\vec{\Delta} + \vec{\Omega}_R) \times \vec{R}$$ Bloch equation

$\vec{R}$: Bloch vector

$$\begin{cases} \frac{dR_x}{dt} = \Omega_R R_z - (-\Delta) R_y \\ \frac{dR_y}{dt} = (-\Delta) R_x \\ \frac{dR_z}{dt} = -\Omega_R R_x \end{cases}$$

对于简单的初始条件，不必解方程，直接从图里面也可以看出来。

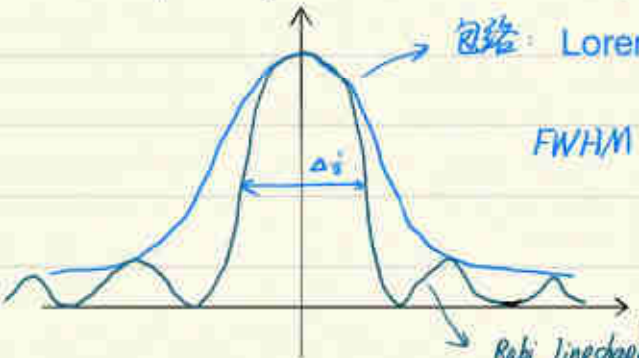
$$R_z = \cos^2\theta + \sin^2\theta \cos(\Omega_{tot} t)$$

$$\sin\theta = \frac{\Omega_R}{\sqrt{\Omega_R^2 + \Delta^2}}, \quad \Omega_{tot} = \sqrt{\Omega_R^2 + \Delta^2}$$

$$\Rightarrow \quad Prob = \frac{1 - R_z}{2} = \frac{1}{2}\frac{\Omega_R^2}{\Omega_R^2 + \Delta^2}\left[1 - \cos\left(\sqrt{\Omega_R^2 + \Delta^2}\, t\right)\right]$$

Rabi Lineshape

选择 π-pulse , $t = \frac{\pi}{\Omega_R}$



$FWHM \sim \Omega_R \sim \frac{1}{t}$

$$\tilde{c}_e := c_e e^{i\omega t}. \tag{5.24}$$
(rotating-frame transformation)

$$c_g(t) = c_g(0)\cos\left(\frac{1}{2}\Omega t\right) - i\tilde{c}_e(0)\sin\left(\frac{1}{2}\Omega t\right)$$
$$\tilde{c}_e(t) = \tilde{c}_e(0)\cos\left(\frac{1}{2}\Omega t\right) - ic_g(0)\sin\left(\frac{1}{2}\Omega t\right)$$

(two-level atom solution, $\Delta = 0$)

as the general solution for the two amplitudes.

Nearly Resonant Interaction

In the case of nonzero detuning Δ, we need to solve Eqs. (5.25). We can again decouple these by differentiating and eliminating appropriate variables, with the result

$$\left(\partial_t^2 - i\Delta\partial_t + \frac{\Omega^2}{4}\right)c_g = 0$$
$$\left(\partial_t^2 - i\Delta\partial_t + \frac{\Omega^2}{4}\right)\tilde{c}_e = 0.$$

Rewriting the decoupled equations as

$$\left(\partial_t - i\frac{\Delta}{2} + i\frac{\tilde{\Omega}}{2}\right)\left(\partial_t - i\frac{\Delta}{2} - i\frac{\tilde{\Omega}}{2}\right)c_g = 0$$
$$\left(\partial_t - i\frac{\Delta}{2} + i\frac{\tilde{\Omega}}{2}\right)\left(\partial_t - i\frac{\Delta}{2} - i\frac{\tilde{\Omega}}{2}\right)\tilde{c}_e = 0,$$

where $\tilde{\Omega}$ is the **generalized Rabi frequency**,

$$\tilde{\Omega} := \sqrt{\Omega^2 + \Delta^2},$$

it is easy to see that any function that causes either factor to vanish will solve the equation, and thus the solutions are linear combinations of functions of the form $\exp(\pm i\Delta t/2 \pm i\tilde{\Omega}t/2)$. We will thus write the solutions as

$$c_g(t) = e^{i\Delta t/2}\left[A_g\cos\left(\frac{1}{2}\tilde{\Omega}t\right) + B_g\sin\left(\frac{1}{2}\tilde{\Omega}t\right)\right]$$
$$\tilde{c}_e(t) = e^{i\Delta t/2}\left[A_e\cos\left(\frac{1}{2}\tilde{\Omega}t\right) + B_e\sin\left(\frac{1}{2}\tilde{\Omega}t\right)\right].$$

Setting $t = 0$ in these equations gives

$$A_g = c_g(0), \qquad A_e = \tilde{c}_e(0),$$

while differentiating the solutions and comparing to the equations of motion gives

$$\partial_t c_g(0) = i\frac{\Delta}{2}c_g(0) + \frac{\tilde{\Omega}}{2}B_g = -i\frac{\Omega}{2}\tilde{c}_e(0) \qquad \Longrightarrow B_g = -\frac{i}{\tilde{\Omega}}\left[\Delta c_g(0) + \Omega\tilde{c}_e(0)\right]$$
$$\partial_t\tilde{c}_e(0) = i\frac{\Delta}{2}\tilde{c}_e(0) + \frac{\tilde{\Omega}}{2}B_e = i\Delta\tilde{c}_e(0) - i\frac{\Omega}{2}\tilde{c}_e(0) \Longrightarrow B_e = \frac{i}{\tilde{\Omega}}\left[\Delta\tilde{c}_e(0) - \Omega c_g(0)\right].$$

Thus, the general solution in terms of initial conditions reads

$$c_g(t) = e^{i\Delta t/2}\left[c_g(0)\cos\left(\frac{1}{2}\tilde{\Omega}t\right) - \frac{i}{\tilde{\Omega}}\left[\Delta c_g(0) + \Omega c_e(0)\right]\sin\left(\frac{1}{2}\tilde{\Omega}t\right)\right]$$
$$\tilde{c}_e(t) = e^{i\Delta t/2}\left[\tilde{c}_e(0)\cos\left(\frac{1}{2}\tilde{\Omega}t\right) + \frac{i}{\tilde{\Omega}}\left[\Delta\tilde{c}_e(0) - \Omega c_g(0)\right]\sin\left(\frac{1}{2}\tilde{\Omega}t\right)\right].$$

(two-level atom solution, arbitrary Δ)

4.4. Dressed States

Dressed States

One thing that we can conlude from the Rabi-flopping behavior is that the old eigenstates $|g\rangle$ and $|e\rangle$ a no longer eigenstates of the coupled system. However, we can still find the new eigenstates. We start writing the equations of motion (5.23) for the coefficients in the matrix form

$$\partial_t \begin{bmatrix} \tilde{c}_e \\ c_g \end{bmatrix} = -i \begin{bmatrix} -\Delta & \Omega/2 \\ \Omega/2 & 0 \end{bmatrix} \begin{bmatrix} \tilde{c}_e \\ c_g \end{bmatrix} = -\frac{i}{\hbar}\tilde{H} \begin{bmatrix} \tilde{c}_e \\ c_g \end{bmatrix},$$

where we identify the rotating-frame Hamiltonian

$$\tilde{H} = (\tilde{H}_A + \tilde{H}_{AF}) = \hbar \begin{bmatrix} -\Delta & \Omega/2 \\ \Omega/2 & 0 \end{bmatrix}$$

in the uncoupled energy basis. We leave the diagonalization of this Hamiltonian as an exercise, but it c be shown that the eigenvalues are

$$E_\pm = -\frac{\hbar\Delta}{2} \pm \frac{\hbar\tilde{\Omega}}{2}, \qquad \text{(dressed-state energi}$$

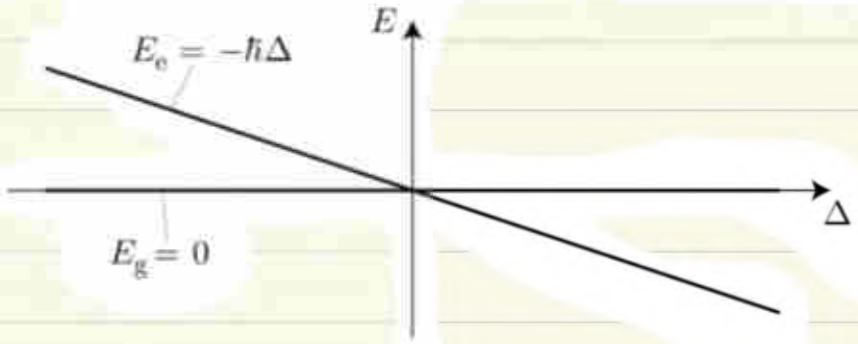
and the corresponding eigenvectors are given by an effective rotation of the uncoupled states,

$$\begin{aligned} |+\rangle &= \sin\theta|g\rangle + \cos\theta|e\rangle \\ |-\rangle &= \cos\theta|g\rangle - \sin\theta|e\rangle, \end{aligned} \qquad \text{(dressed stat}$$

where by convention the state $|+\rangle$ has the higher energy, and the **Stückelberg angle** θ is defined via

$$\tan 2\theta = -\frac{\Omega}{\Delta} \quad \left(0 \le \theta < \frac{\pi}{2}\right). \qquad \text{(Stückelberg ang}$$

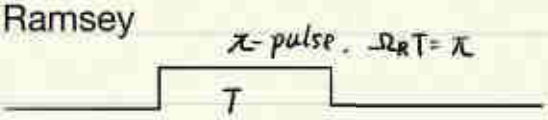
These are the **dressed states** of the atom, and we see from Eq. (5.64) that the coupling to the field cau an **avoided crossing** in the energy level structure of the atom. That is, in the uncoupled case, the energ of the ground and excited states—the **bare states**—are 0 and $-\hbar\Delta$, respectively. The energy curves cr when $\Delta = 0$.



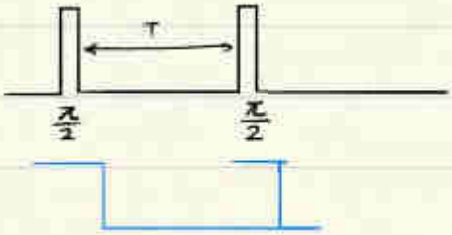
4.5 Ramsey Method

I I Rabi的学生：Norman Ramsey

Rabi的办法：



Ramsey的办法：



包络会变得非常宽

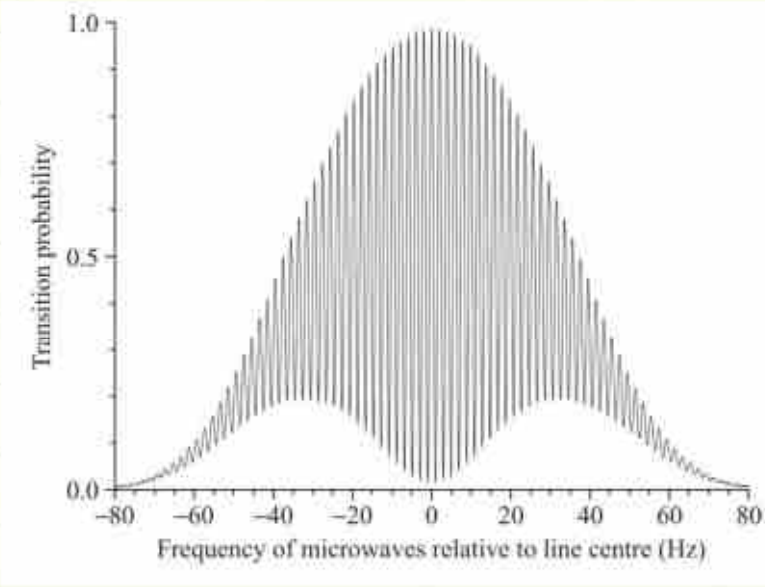
这两个光的相位是相同的（为了保证沿着相同的方向

在T的时间内，在xOy平面内转动的角度为： $\theta = \Delta \cdot T$

故完成这个流程之后，有： $Prob = \frac{1-R_z}{2} = \frac{1+\cos(\Delta \cdot T)}{2}$

Ramsey Lineshape： $FWHM \propto \frac{1}{T}$

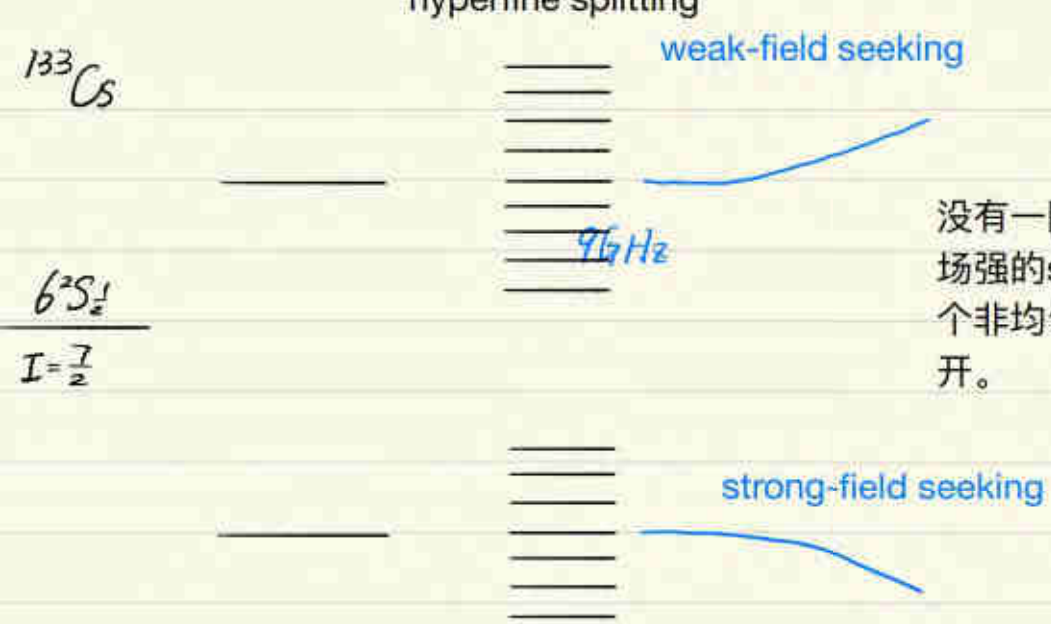
Rabi方法中，需要保证Omega_R在整个过程中都保持稳定。因为Rabi方法里面，半高全宽反比于打pi脉冲的时间，所以不能把Omega_R调大让他快一点，否则线宽就会变很宽。但是Ramsey方法中间是自由演化的过程，两边是pi/2的光，可以把两边的pi/2的对应的Omega_R变得很大，让时间变得短，而不影响线宽。（线宽仍然取决于中间的T。



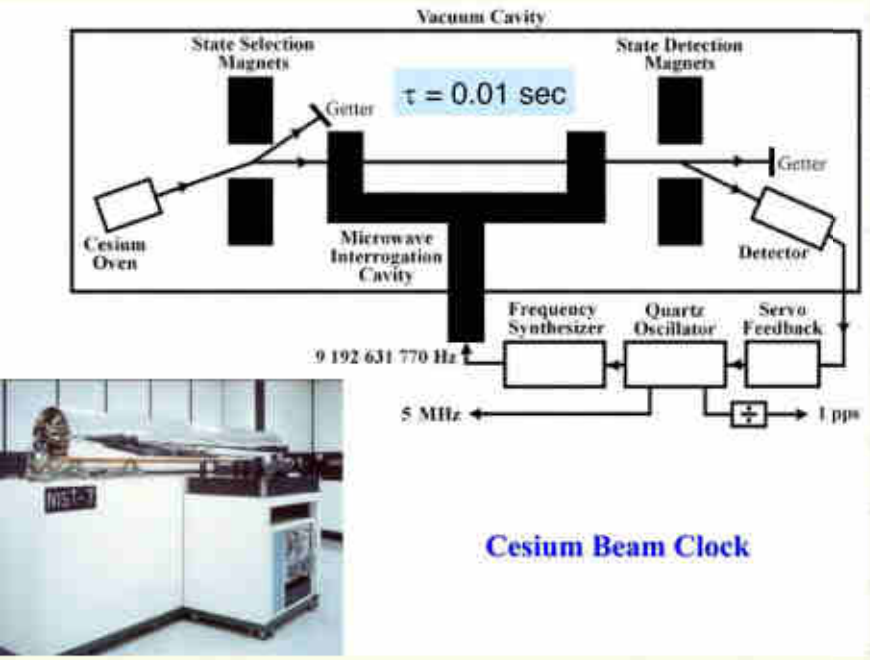
Adiabatic fast passage

把频率调节到远失谐： $\begin{cases} -\Delta \ll D \\ |-\Delta| \gg \Omega_R \end{cases}$

然后扫描，令 $-\Delta$ 从 $-\infty \to +\infty$



没有一阶效应，但是有二阶效应。对场强的seeking过程不同，所以经过一个非均匀磁场后，两个不同的态会分开。



左边，右边的pi/2脉冲可以加一个pi/2的相位差。这样就可以把Ramsey的fringe挪一下，到一个斜坡上面。

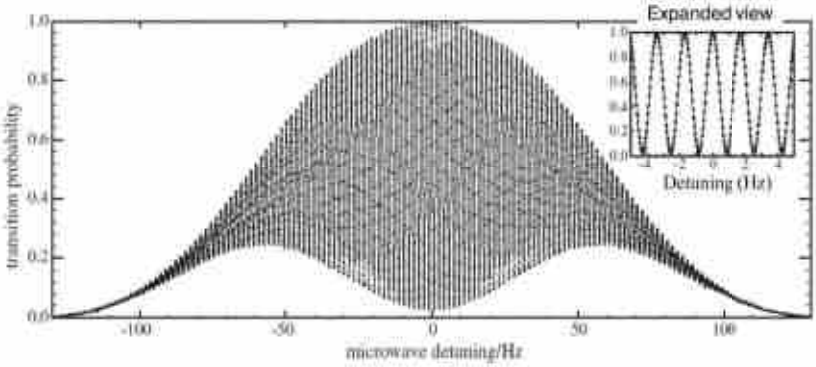
使用Ramsey方法，半高全宽很窄，所以能做的很精确。

中间加微波，导致原子跃迁。

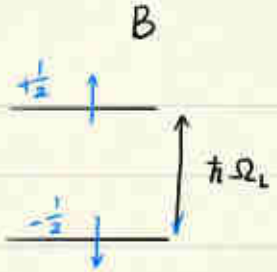
Separated oscillatory field method = Ramsey method

Norman F. Ramsey
Nobel Prize in Physics, 1989
"for the invention of the separated oscillatory fields method and its use in the hydrogen maser and other atomic clocks"

Ramsey Fringes of a Cesium Atomic Clock



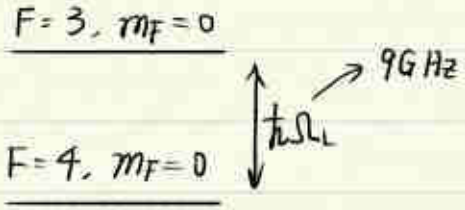
NMR



B_T

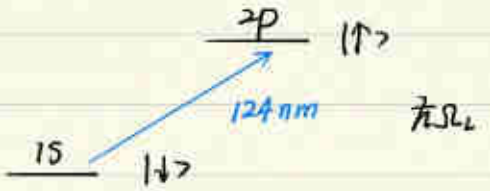
$$\Omega_R = \frac{2\mu B_T}{\hbar}$$

^{133}Cs



$$\Omega_R = \langle F=4, m_F=0 | \frac{\vec{\mu}\cdot\vec{B}_{rad}}{\hbar} | F=3, m_F=0 \rangle$$

习惯上，也可以称为是一对spin up 和spin down



$$\Omega_R = \langle 1S | \frac{e\vec{r}\cdot\vec{E}_{rad}}{\hbar} | 2p \rangle$$

4.6. Optical Bloch Equation

T1: Longitudinal在初始化之后，慢慢变乱的时间 } 一般 $T_2 < T_1$

T2: 横向的

当 measurement time $\gg T_1, T_2$ 需要考虑退相干

Bloch $R_z = 1$

$|1s\rangle$

$$\begin{cases} \dfrac{dR_x}{dt} = \Omega_R \Omega_z + \Delta R_y - \dfrac{\Gamma}{2} R_x \\ \dfrac{dR_y}{dt} = -\Delta R_x - \dfrac{\Gamma}{2} R_y \\ \dfrac{dR_z}{dt} = -\Omega_R R_x - \underline{\Gamma (R_z - 1)} \end{cases}$$

当 $R_z = 1$，表示没有力 0

$|2p\rangle$

自发辐射速率：Γ

（$\frac{\Gamma}{2}$ 中 $\frac{1}{2}$ 的原因是，$a|1s\rangle + b|2p\rangle$，$R_x = 2\,\mathrm{Re}(a^* b)$，$|b|^2_{t=t} = |b|^2_{t=0}\, e^{-\Gamma t} \Rightarrow |b|_t = |b|_0\, e^{-}$

当达到平衡后，得到的方程称为Optical Bloch Equation：

1. 考虑了退相干；
2. 考虑平衡态。

$$\begin{cases} 0 = \Omega_R \Omega_z + \Delta R_y - \dfrac{\Gamma}{2} R_x \\ 0 = -\Delta R_x - \dfrac{\Gamma}{2} R_y \\ 0 = -\Omega_R R_x - \underline{\Gamma (R_z - 1)} \end{cases}$$

Transition Probability: $n_e = Prob = \frac{1}{2}\frac{1}{1+\frac{\Gamma^2}{2\Omega_R^2}\left[1+\left(\frac{2\Delta}{\Gamma}\right)^2\right]}$

$$\Omega_R = \frac{e\boxed{\langle g|\vec{r}|e\rangle}\cdot\boxed{\vec{E}_{rad}}}{\hbar}$$

理论 实验

所以重新定义: $\frac{\Gamma^2}{2\Omega_R^2} = \frac{I_{sat}}{I}$ → Saturation Intensity, 与原子跃迁相关的参数

$$\Rightarrow \quad n_e = Prob = \frac{1}{2}\frac{1}{1+\frac{I_{sat}}{I}\left[1+\left(\frac{2\Delta}{\Gamma}\right)^2\right]}$$

$$n_e = \frac{\frac{\Omega^2}{4}}{\Delta^2+\frac{\Omega^2}{2}+\frac{\Gamma}{2}} \qquad , \quad I_{sat} = \frac{\pi}{3}\frac{hc}{\lambda^3\tau}$$

$$= \frac{1}{2}\frac{\frac{I}{I_{sat}}\Gamma}{\left(1+\frac{I}{I_{sat}}\right)\Gamma^2+4\Delta^2}$$

散射率会接近 $\frac{\Gamma}{2}$

每个原子的亮度不会一直升高，存在一个饱和值

$\Gamma' = \Gamma\sqrt{1+\frac{I}{I_{sat}}}$ 吸收的曲线会变矮，因此导致线宽变宽。(蓝色)

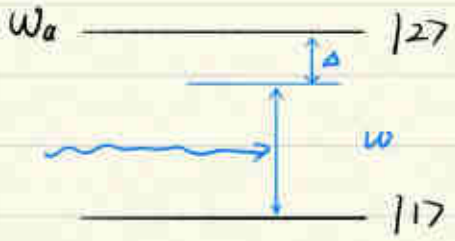
原子的跃迁会被激光饱和

通过这个方法，上态最大的population只能是1/2

截面 $\frac{n_e}{\tau} = \frac{I}{h\nu}\sigma = \frac{I}{2I_{sat}}\frac{1}{\tau}$

$$\Rightarrow \quad \sigma = \frac{h\nu}{2I_{sat}}\frac{1}{\tau} \sim \frac{\lambda^2}{2}$$

与入射光波长有关



$$H_{int} = -\vec{d}\cdot\vec{E}\ .$$

$$\vec{d} = |1\rangle\langle 2|\vec{\mu}_{12} + |2\rangle\langle 1|\vec{\mu}_{21}\ ,\quad \vec{\mu}_{ij} = \langle i|\vec{d}|j\rangle$$

$$H = \hbar\omega_a |2\rangle\langle 1| - \left(|1\rangle\langle 2|\mu_{12} + |2\rangle\langle 1|\mu_{21}\right)\left(\mathcal{E}e^{-i\omega t} + \mathcal{E}^* e^{i\omega t}\right)$$

不考虑耗散，还是一个纯态

$$|\psi\rangle = C_1(t)|1\rangle + C_2(t)|2\rangle\ ,\quad |C_1(t)|^2 + |C_2(t)|^2 = 1$$

$$\begin{cases} i\hbar\dot{C}_2 = \hbar\omega C_2 - \frac{1}{2}\left(\mathcal{E}e^{-i\omega t} + c.c.\right)\mu_{21}C_1 \\ i\hbar\dot{C}_1 = -\frac{1}{2}\left(\mathcal{E}e^{-i\omega t} + c.c.\right)\mu_{12}C_2 \end{cases}$$

做变换 $C_2(t) = \tilde{C}_2(t)e^{-i\omega t}$ 相当于变到rotating-frame

$$\Rightarrow \begin{cases} i\hbar\dot{\tilde{C}}_2 = -\hbar\Delta C_2 - \frac{1}{2}\left(\mathcal{E} + \mathcal{E}^* e^{i2\omega t}\right)\mu C_1 \\ i\hbar\dot{C}_1 = -\frac{1}{2}\left(\mathcal{E}e^{-2i\omega t} + \mathcal{E}^*\right)\mu\tilde{C}_2 \end{cases}$$

Rotating wave approximation. 条件: $\omega, \omega_a \gg \Delta, \Omega$

定义Rabi Frequency: $\frac{\mathcal{E}\mu}{\hbar} = \Omega$

$$\Rightarrow \begin{cases} i\dot{\tilde{C}}_2 = -\Delta C_2 - \frac{1}{2}\Omega C_1 \\ i\dot{C}_1 = -\frac{1}{2}\Omega^* C_2 \end{cases}$$

解: $\begin{cases} C_1(t) = \left\{\cos\left(\frac{\Omega'}{2}t\right) - i\frac{\Delta}{\Omega'}\sin\left(\frac{\Omega'}{2}t\right)\right\}e^{i\frac{\Delta}{2}t} \\ C_2(t) = i\frac{\Omega}{\Omega'}\sin\left(\frac{\Omega'}{2}t\right)e^{i\frac{\Delta}{2}t} \end{cases}$ $\Omega' = \sqrt{\Omega^2 + \Delta^2}$

Population: $|C_2|^2 = \left(\frac{\Omega}{\Omega'}\right)^2\sin^2\left(\frac{1}{2}\Omega' t\right)$

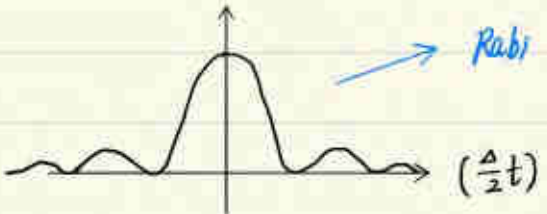
$|C_1|^2 = 1 - |C_2|^2$

当 $\omega \gg \Delta \gg \Omega$ 时,

$$|C_1(t)|^2 = 1$$

$$\begin{cases} i\dot{\tilde{C}}_2 = -\Delta\tilde{C}_2 - \frac{1}{2}\Omega C_1 \\ i\dot{C}_1 = -\frac{\Omega}{2\Delta}\left(1 - e^{i\Delta t}\right) \approx i\frac{\Omega}{\Delta}\sin\left(\frac{\Delta}{2}t\right)e^{i\frac{\Delta}{2}t}\ ,\quad \frac{\Omega}{\Delta} \ll 1 \end{cases}$$

$$|C_2(t)|^2 = \frac{1}{4}\Omega^2 t^2\,\mathrm{sinc}\left(\frac{\Delta}{2}t\right)$$



这个模型本来就是近似，所以粒子数不守恒

$\Delta \gg \Omega$

令 $\dot{\tilde{C}}_2 = 0$, $\Rightarrow 0 = -\Delta \tilde{C}_2 - \frac{1}{2}\Omega C_1 \quad \Rightarrow \tilde{C}_2 = -\frac{\Omega}{2\Delta} C_1$

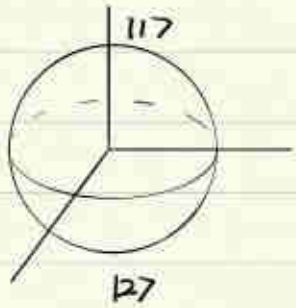
$\Rightarrow i\dot{C}_1 = -\frac{1}{2}\Omega C_2 \quad \Rightarrow C_1 \approx C_1(0)\, e^{-i\frac{\Omega}{4\Delta}t}$

Ramsey: $C_2 \to -\frac{\Omega}{2\Delta}(1-e^{-i\Delta\tau_p})$

$- \frac{\Omega}{2\Delta}(1-e^{-i\Delta\tau_p})\, e^{-i\Delta T}$

最终: $C_2 = -\frac{\Omega}{2}\left\{\frac{1-e^{-i\Delta\tau_p}}{\Delta} e^{-i\Delta T} + \frac{1-e^{-i\Delta\tau_p}}{\Delta}\right\}$

$|C_2|^2 = \frac{1}{4}\Omega^2\tau_p^2 \operatorname{sinc}\left(\frac{\Delta\tau_p}{2}\right)^2 \cos^2\left(\frac{\Delta T}{2}\right)$



原始 Hamiltonian: $H = \hbar\omega_a |2\rangle\langle 2| - \frac{1}{2}\left\{\Omega e^{i\omega t}|1\rangle\langle 2| + h.c.\right\}$

$= H_0 + V$

$H_I = e^{iH_0 t} V e^{-iH_0 t}$

$= -\Delta |2\rangle\langle 2| - \frac{1}{2}\left\{\Omega |1\rangle\langle 2| + h.c.\right\}$

$H_I = \begin{pmatrix} -\Delta & -\frac{1}{2}\Omega \\ -\frac{1}{2}\Omega & 0 \end{pmatrix}$

$$\Rightarrow \begin{cases} |+\rangle = \begin{pmatrix} \frac{\Delta - \sqrt{\Delta^2+\Omega^2}}{\Omega} \\ 1 \end{pmatrix} = \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix} \to \varepsilon_+ = \frac{1}{2}\left(-\Delta + \sqrt{\Delta^2+\Omega^2}\right) \\ |-\rangle = \begin{pmatrix} \frac{\Delta + \sqrt{\Delta^2+\Omega^2}}{\Omega} \\ 1 \end{pmatrix} = \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix} \to \varepsilon_- = \frac{1}{2}\left(-\Delta - \sqrt{\Delta^2+\Omega^2}\right) \end{cases}$$

$\Rightarrow \quad \tan 2\theta = -\frac{\Omega}{\Delta}$

4.1 Adiabatic Passage

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where we identify the rotating-frame Hamiltonian

$$\tilde{H} = (\tilde{H}_A + \tilde{H}_{AF}) = \hbar \begin{bmatrix} -\Delta & \Omega/2 \\ \Omega/2 & 0 \end{bmatrix}$$

in the uncoupled energy basis. We leave the diagonalization of this Hamiltonian as an exercise, but it can be shown that the eigenvalues are

$$E_\pm = -\frac{\hbar\Delta}{2} \pm \frac{\hbar\tilde{\Omega}}{2}, \qquad \text{(dressed-state energies)}$$

and the corresponding eigenvectors are given by an effective rotation of the uncoupled states,

$$|+\rangle = \sin\theta|g\rangle + \cos\theta|e\rangle$$
$$|-\rangle = \cos\theta|g\rangle - \sin\theta|e\rangle, \qquad \text{(dressed states)}$$

原始 Hamiltonian: $H = \hbar\omega_0 |2\rangle\langle 2| - \frac{1}{2}\{\Omega e^{i\omega t}|1\rangle\langle 2| + h.c.\}$

$$= H_0 + V$$

$$H_I = e^{iH_0 t} V e^{-iH_0 t}$$

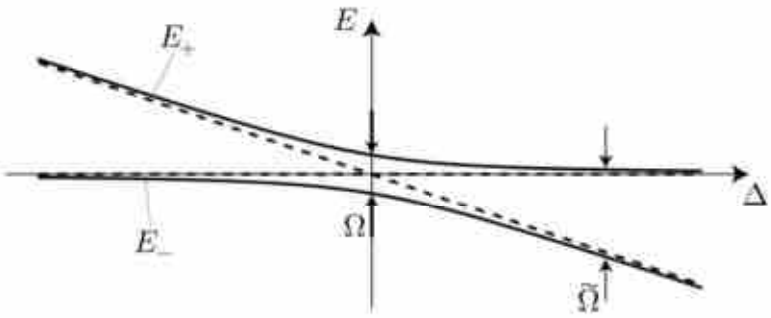
$$= -\Delta |2\rangle\langle 2| - \frac{1}{2}\{\Omega |1\rangle\langle 2| + h.c.\}$$

$$H_I = \begin{pmatrix} -\Delta & -\frac{1}{2}\Omega \\ -\frac{1}{2}\Omega & 0 \end{pmatrix}$$

$$\Rightarrow \begin{cases} |+\rangle = \begin{pmatrix} \frac{\Delta - \sqrt{\Delta^2+\Omega^2}}{\Omega} \\ 1 \end{pmatrix} = \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix} \rightarrow \varepsilon_+ = \frac{1}{2}(-\Delta + \sqrt{\Delta^2+\Omega^2}) \\ |-\rangle = \begin{pmatrix} \frac{\Delta + \sqrt{\Delta^2+\Omega^2}}{\Omega} \\ 1 \end{pmatrix} = \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix} \rightarrow \varepsilon_- = \frac{1}{2}(-\Delta - \sqrt{\Delta^2+\Omega^2}) \end{cases}$$

$$\tan 2\theta = -\frac{\Omega}{\Delta}$$

The coupling between the two levels lifts the degeneracy, however, converting the level crossing into a hyperbolic avoided crossing. Avoided crossings happen commonly in quantum mechanics, and here we have a simple model for this phenomenon.



In the limit of large detuning, when the coupling is small, we can approximately identify the coupled eigenstates with the uncoupled eigenstates. Near resonance, however, the states are mixed, and the energies are shifted. The energy shifts are the **ac Stark shifts**, or **lamp shifts**, which we will treat in more detail later.

$\Delta = \alpha t$

in the limit $t \longrightarrow \infty$. Thus, the fraction that *didn't* adiabatically follow the dressed state is

$$P_{\text{lost}} = e^{-2\pi|\nu|} = \exp\left(-\frac{\pi\Omega^2}{2|\alpha|}\right) = \exp\left(-\frac{\pi\Omega^2}{2|\partial_t\Delta|}\right).$$

(Landau–Zener tunnel probability) (5.96)

This is the Landau–Zener result. In the limit of a strong field and slow sweep ($\Omega^2 \gg |\partial_t\Delta|$), nothing is lost—all the population adiabatically follows the dressed state and makes the transition. In the opposite regime of a weak field and fast sweep ($\Omega^2 \ll |\partial_t\Delta|$), the population jumps (tunnels) across the gap, and everything stays in the original state.

Hamiltonian含时:

② $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)\frac{\partial}{\partial t}|\psi(t)\rangle$, $H(t)|\phi_n(t)\rangle = E_n(t)|\phi_n(t)\rangle$ ①

$\Rightarrow$ ③ $|\psi(t)\rangle = \sum_n C_n(t)|\phi_n(t)\rangle e^{i\theta_n(t)}$, $\theta_n(t) = -\frac{i}{\hbar}\int_0^t E_n(t')dt'$

$i\hbar\sum_n\left(\dot{C}_n(t)|\phi_n(t)\rangle + C_n(t)|\dot{\phi}_n(t)\rangle + \cancel{\dot{\theta}_n C_n(t)|\phi_n(t)\rangle}\right)e^{i\theta_n(t)} = \cancel{C_n E_n e^{i\theta_n(t)}|\phi_n(t)\rangle}$

$\Rightarrow \sum_n \dot{C}_n(t)|\phi_n(t)\rangle e^{i\theta_n(t)} = -\sum_n C_n(t)|\dot{\phi}_n(t)\rangle e^{i\theta_n(t)}$

$\langle\phi_m(t)|$ 作用:

$\Rightarrow \dot{C}_m(t) = -\sum_n C_n(t)\langle\phi_m(t)|\dot{\phi}_n(t)\rangle e^{i\theta_n(t)}$ ④

① 求导 $\Rightarrow \dot{H}(t)|\phi_n(t)\rangle + H(t)|\dot{\phi}_n(t)\rangle = \dot{E}_n(t)|\phi_n(t)\rangle + E_n(t)|\dot{\phi}_n(t)\rangle$

左乘 $\langle\phi_m(t)|$,

$\Rightarrow \langle\phi_m(t)|\dot{H}|\phi_n(t)\rangle + E_m(t)\langle\phi_m(t)|\dot{\phi}_n(t)\rangle = \dot{E}_n(t)\delta_{mn} + E_n(t)\langle\phi_m(t)|\dot{\phi}_n(t)\rangle$

$\Rightarrow \langle\phi_m(t)|\dot{H}|\phi_n(t)\rangle = (E_n(t) - E_m(t))\langle\phi_m(t)|\dot{\phi}_n(t)\rangle$ ⑤

⑤代入④: $\dot{C}_m(t) = -C_m(t)\langle\phi_m|\dot{\phi}_m(t)\rangle - \sum_{n\neq m} C_n(t)\frac{\langle\phi_m(t)|\dot{H}|\phi_n(t)\rangle}{E_n(t) - E_m(t)}$

绝热条件: $\left|\frac{\hbar\langle\phi_m(t)|\dot{H}|\phi_n(t)\rangle}{(E_n - E_m)^2}\right| \ll 1$, $\Leftrightarrow \left|\frac{\hbar\langle\phi_m(t)|\dot{\phi}_n(t)\rangle}{E_n - E_m}\right| \ll 1$

绝热近似下: $C_m(t) = C_m(0)e^{i\gamma_m(t)}$, $\gamma_m(t) \equiv i\int_0^t\langle\phi_m(t')|\dot{\phi}_m(t')\rangle dt'$

Berry phase (Geometric pha

即 $|\psi(t)\rangle = C_n(0)e^{i\theta_n(t)}e^{i\gamma_n(t)}|\phi_n(t)\rangle$

刚开始处在第n个本征态上面

对Berry Phase的讨论：

(1) 如果参量 R 是标量

$$\frac{\partial \phi_n}{\partial t} = \frac{\partial \phi_n}{\partial R}\frac{dR}{dt}, \quad \gamma_n(t) = i\int_0^t \langle \phi_n(t') | \frac{\partial \phi_n}{\partial R} \rangle \frac{dR}{dt'} dt$$

$$= i\int_{R_i}^{R_f} \langle \phi_n(t') | \frac{\partial \phi_n}{\partial R} \rangle dR$$

当 $R_i = R_f$，$\gamma_n(t) = 0$

(2) 如果参量 R 是矢量 $\vec{R} = (R_1, R_2, \cdots, R_s)$

$$\frac{\partial \phi_n}{\partial t} = \sum_i \frac{\partial \phi_n}{\partial R_i}\frac{dR_i}{dt} = (\nabla_R \phi_n)\frac{d\vec{R}}{dt}$$

$$\Rightarrow \gamma_n(t) = i\int_{\vec{R}_i}^{\vec{R}_f} \langle \phi_n | \nabla_R \phi_n \rangle d\vec{R}$$

当 $\vec{R}_i = \vec{R}_f$，有可能相差一个相位.

Chapter 5 碱金属原子：Alkali metal

氢原子能量关于l的简并性：

$$V(r) \sim -\frac{k}{r} \quad , \quad SO(4)$$

多一个守恒量：拉普拉斯-龙格-楞次矢量：

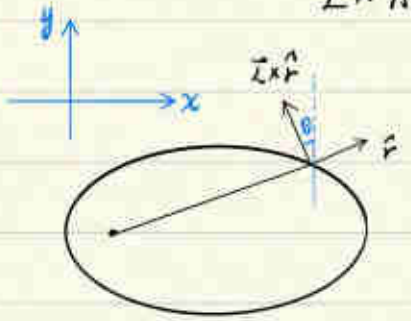
$$\vec{A} = \vec{p}\times\vec{L} - mk\frac{\vec{r}}{r} = \vec{p}\times\vec{L} - mk\hat{r}$$

偏心率 $e = \frac{|\vec{A}|}{mk}$

Laplace-Runge-Lentz

$$\vec{L}\times\vec{A} = \vec{L}\times(\vec{p}\times\vec{L}) - mk\vec{L}\times\frac{\vec{r}}{r}$$

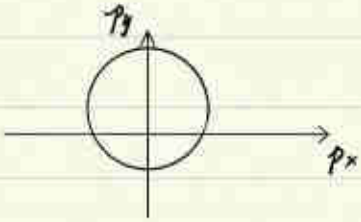
$$= L^2\vec{p} - mk\frac{\vec{r}}{r}$$



$$\begin{cases} 0 = L^2 p_x - Lmk\sin\theta & (x\text{ 方向}) \\ \vec{L}\cdot\vec{A} = L^2 p_y - Lmk\cos\theta & (y\text{ 方向}) \end{cases}$$

$$\Rightarrow \quad p_x^2 + \left(p_y - \frac{A}{L}\right)^2 = \frac{m^2k^2}{L^2}$$

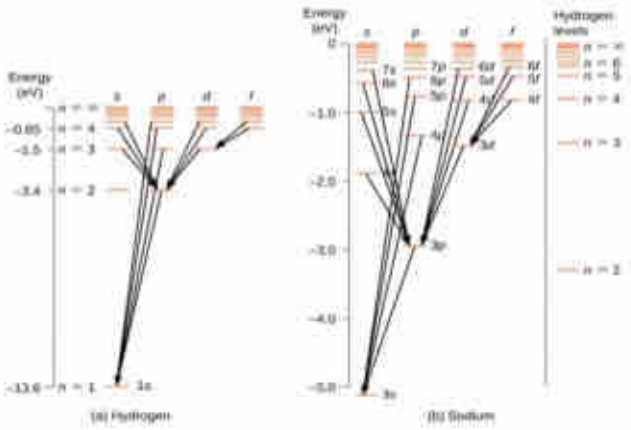
Hodograph.



$$\vec{u} = p_0\frac{p^2-p_0^2}{p^2+p_0^2}\hat{u}_4 + p_0\frac{2p_0}{p^2+p_0^2}\vec{p}$$

量子数亏损

能级的简并来源于库伦势。发生退简并之后，说明库伦势不再能描述它。



Values of quantum defect for sodium

l	$n=3$	$n=4$	$n=5$	$n=6$
0	1.373	1.357	1.352	1.349
1	0.883	0.867	0.862	0.859
2	0.010	0.011	0.013	0.011
3		0.000	-0.001	-0.008

TABLE 11.1. Quantum defects of the alkali atoms for $\ell = 0-3$.

ℓ	Li	Na	K	Rb	Cs
s	0.40	1.35	2.19	3.13	4.06
p	0.04	0.85	1.71	2.66	3.59
d	0.00	0.01	0.25	1.34	2.46
f	0.00	0.00	0.00	0.01	0.02

自旋轨道相互作用

$V \rightarrow V_{pen} + V_{pol} + V_{so}$

电子穿进去；极化的贡献（这个电荷对其他负电荷的作用），

l 较小显著　　l 较大显著

$$R_{nl}(r) = \frac{u_{nl}(r)}{r}$$

$$\left[-\frac{\hbar^2}{2m_e}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2m_e r^2} + V(r)\right] u_{nl}(r) = E_{nl} u_{nl}(r)$$

1D- Schroedinger Eq.

$$V_{eff}(r) = V(r) + \frac{\ell(\ell+1)\hbar^2}{2m_e r^2}$$

$$R_{nl}(r) = -\left[\frac{(n-l-1)!}{2n[(n+l)!]^3}\right]^{\frac{1}{2}} \left(\frac{2Z}{nm_e}\right)^{l+\frac{3}{2}} r^l e^{-\frac{Zr}{nm_e}} L_{n-l-1}^{2l+1}\left(\frac{2Zr}{nm_e}\right)$$

10.2.1 量子缺陷（Quantum Defacts）-- 碱金属光谱的概括

所谓碱金属，是指最外层1个电子，内部满壳层的情况。比惰性气体多出1个电子因此，它的电离能显著地低于惰性气体。对于碱金属的光谱来说，我们发现可以用如下的公式来表达就可以解释它的粗结构：

$$E = \frac{-Rhc}{(n-\delta_l)^2}$$

这里，δ_l 就是 **量子缺陷**(quatum defact). 一般来说，它只与轨道角动量 l 有关，与n关系很小。而且 l 越大，缺陷约小。下表是钠的量子缺陷：

$l \setminus n$ 3456 01.3731.3571.3521.349 10.8830.8670.8620.859 20.0100.0110.0120.011 3-0.000-0.001-0.008

因此，量子缺陷常常总结成如下的式子：

$$\delta_s = 1.35, \qquad \delta_p = 0.86, \qquad \delta_d = 0.01, \qquad \delta_{l>2} \simeq 0.00$$

下面，我们尝试去解释为什么会是这样（与n无关，与l有关，$n-\delta$ 的形式）

1. penetration：

10.2.2 有效核电荷数解释

我们是这样理解一个碱金属的：当最外层电子的离核距离比较远的时候，它感受到的核电荷数是1. 但是当它的离核距离比较近的时候（进入内层电子的区域）它会感受到更大的核电荷数直到Z。因此，它的势能是：

$$\begin{aligned} r \to \infty, \qquad & V(r) \to -1/r \\ r \to 0, \qquad & V(r) \to -Z/r \end{aligned}$$

这里其实表达的是**中心场近似（central-field approximation）**，认为内部电子的分布是中心对称的，因此内层电子对价电子的作用也是中心对称的。于是，我们也会把这样的势能表达成：

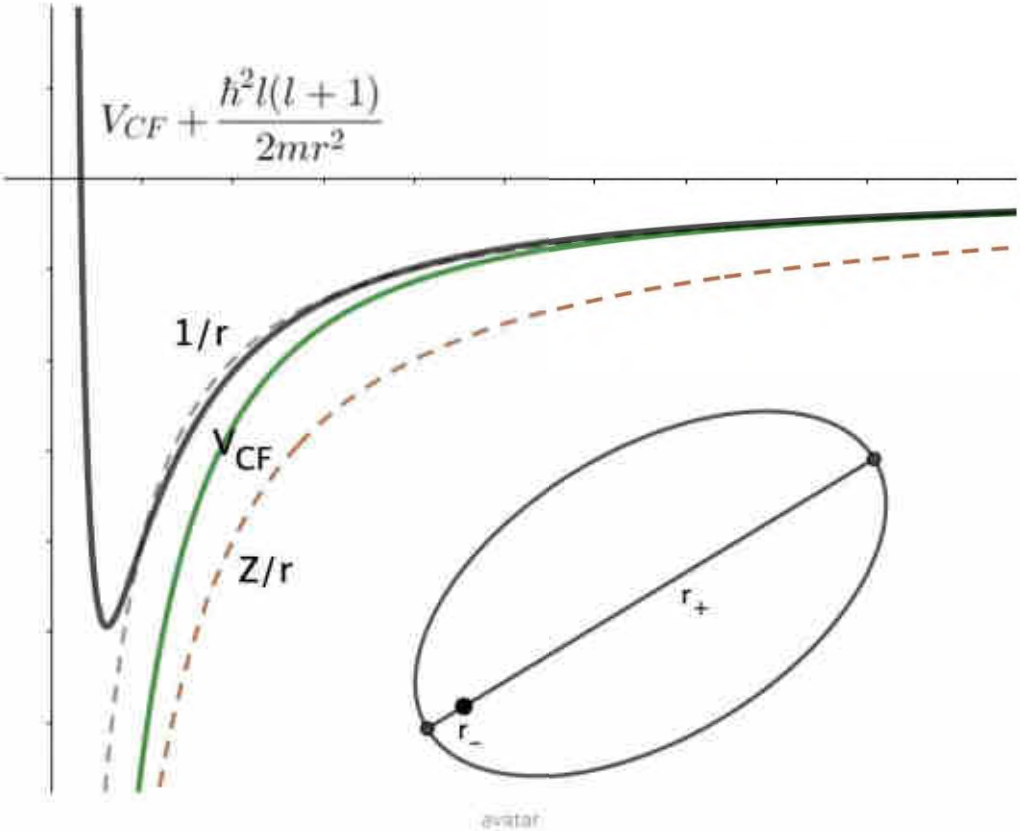
$$V(r) = -\frac{Z(r)}{r}$$

因此在径向方向的分布函数是（类氢原子）$|P(r)| = |rR_{nl}(r)|^2$ 满足：

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{CF}(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right\} P(r) = EP(r)$$

可以看到，整体的势能会带有一项"离心力项"(centrifugal barier)，它阻止了当 $l > 0$ 时电子到

达 $r=0$ 处.



在这种势能下，电子的轨迹会是一个椭圆。如果我去求这个椭圆的“近日点”和“远日点”，我们会发现(在近似下)

$$-\frac{Rhc}{n^2}=-\frac{e^2/4\pi\epsilon_0}{r}+\frac{\hbar^2 l(l+1)}{2mr^2}$$

$$l\ll n,\quad \begin{cases} r+=2n^2a_0 \\ r-=\frac{1}{2}l(l+1)a_0 \end{cases}$$

在这种近似下，我们发现，“近日点”只与l有关，“远日点”至于n有关。当l很小的时候，离核很近更受影响，而当l变大的时候离核越远。这里解释了为什么当l变大的时候量子缺席越来越小。

10.2.3 径向波函数解释

径向波函数渐进分析

我们仍然利用类氢原子波函数去理解碱金属原子的行为。首先定义一个碱金属原子可用的单位长度 $a_u=a_0m/M$ 。其次，利用渐进分析，我们得到：

$$r\to\infty,\qquad R_{nl}\to r^{n-1}e^{-Zr/na_0}$$
$$r\to 0,\qquad R_{nl}\to r^{l}$$

因此，我们考虑 $|P(r)|=|rR_{nl}(r)|^2$ 的图像的时候：

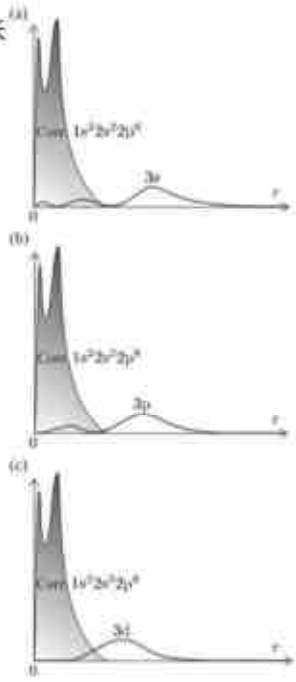
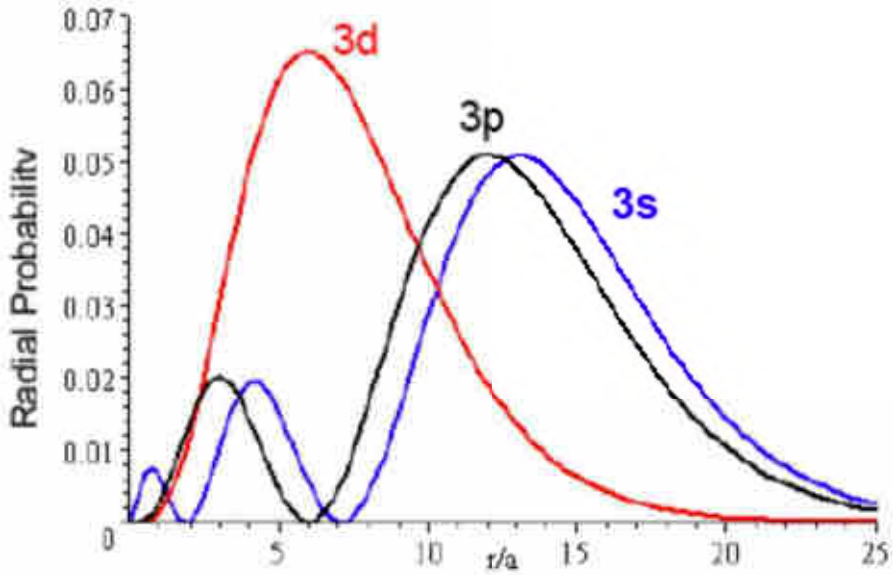


Fig. 4.4 The probability density of the electrons in a sodium atom as a function of r. The electrons in the $n=1$ and $n=2$ shells make up the core, and the probability density of the unpaired outer electron is shown for the $n=3$ shell with $l=0$, 1 and 2. The probability is proportional to $|P(r)|^2=r^2|R(r)|^2$; the r^2 factor accounts for the increase in volume of the spherical shell between r and $r+dr$ (i.e. $4\pi r^2dr$) as the radial distance increases. The decreasing penetration of the core as l increases can be seen clearly—the 3d electrons lies mostly outside the core with a wavefunction and binding energy very similar to those for the 3d configuration in hydrogen. These wavefunctions could be calculated by the simple numerical method described in Exercise 4.10, making the 'frozen core' approximation, i.e. that the distribution of the electrons in the core is not affected by the outer electron—this gives sufficient accuracy to illustrate the qualitative features. (The iterative method described in Section 4.4 could be used to obtain more accurate numerical wavefunctions.)



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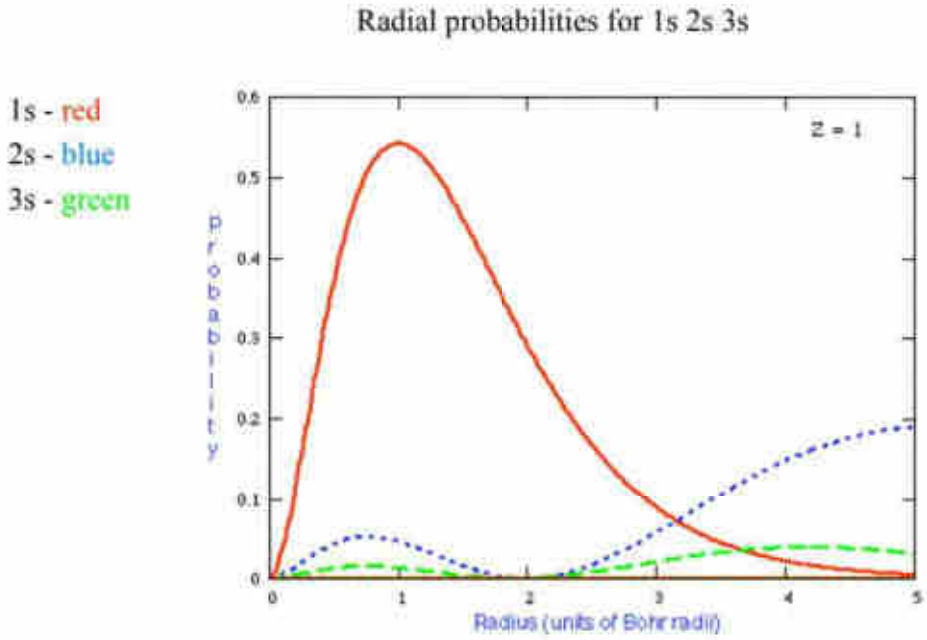
可以看到，s波具有3个波包，p波具有2个波包，d波具有1个波包。s波包在离核很近的时候具有更多的概率。同时，我们注意到，当 l 固定的时候，变化n，$(n \gg l)$，第一个波包的位置几乎不变。

l 不变时，第一个波包位置固定



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这也间接解释了为什么不同的n的量子缺陷是近乎相同的。

10.2.4 微扰论解释

$$\langle r^k \rangle = \int |R_{nl}|^2 r^{k+2} dr \begin{cases} \propto n^{-3}, & k < -1 \\ \propto n^{-2}, & k = -1 \\ \propto n^{2k}, & k > 0 \end{cases}$$

$$\langle \frac{1}{r} \rangle = \frac{Z}{a_\mu n^2}$$

$$\langle \frac{1}{r^2} \rangle = \frac{Z^2}{a_\mu^2 n^3 (l+\frac{1}{2})}$$

$$\langle \frac{1}{r^3} \rangle = \frac{Z^3}{a_\mu^3 n^3 l(l+\frac{1}{2})(l+1)}$$

$$\langle \frac{1}{r^4} \rangle \sim \frac{Z^4}{a^4 n^3 l^5}$$

$$\langle \frac{1}{r^6} \rangle \sim \frac{Z^4}{a^4 n^3 l^9}$$

因此，我们在类氢原子的哈密顿量基础上考虑微扰 $H'(r) = -(Z(r)-1)/r$ 所以，可以得到，

$$\langle -\frac{Z(r)-1}{r} \rangle \propto \frac{1}{n^3}$$

不妨设，$\langle H' \rangle = 2R\delta_l/n^3$ 因此，我们可以得到：

$$E = \frac{R}{n^2} + \frac{2R\delta_l}{n^3} \simeq \frac{R}{(n-\delta_l)^2}$$

10.3.4 相位解释

量子缺陷作为一个相位出现。仍然是利用类氢原子的方程去解释。径向方程为 $P(r) = rR(r)$：

$$\left\{ -\frac{\hbar^2}{2\mu}[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}] - \frac{e^2/4\pi\epsilon_0}{r} - E \right\} P_l(\nu, r) = 0$$

我们这里取两个变量 ν, r. 能量的表达式为

$$E = -\frac{R}{\nu^2}$$

f: regular ; g: irregular

在一般的氢原子解中，$\nu = n$，这是因为上式有两个通解f 和 g:

$$\begin{aligned} r \to 0, \qquad & f \propto r^{l+1}, \qquad g \propto r^{-l} \\ r \to \infty, \qquad & f \to C(r)\sin[\pi(\nu - l)]e^{r/\nu} \\ & g \to C(r)\cos[\pi(\nu - l)]e^{r/\nu} \end{aligned}$$

我们希望 $r \to \infty$ 的时候，f为0。当只考虑氢原子的时候只有f形式。因此，需要 $\nu - l = n'$ 某一个整数。也就是 $\nu = n$. 此时，能量为 $E = -R/n^2$ 与我们得到的氢原子能量一致。

这时候我们希望把上式拓展到碱金属原子。在拓展到碱金属的时候就不仅仅有f形式的解了，也有一部分g函数形式。我们认为这两种形式的占比为 $\cos^2(\pi\delta_l)$ 和 $\sin^2(\pi\delta_l)$ 。因此，新的波函数为：在r很大的时候

$$\begin{aligned} P_l(\nu, r) &= C(r)e^{r/\nu}\{\sin(\pi\delta_l)\cos(\pi(\nu - l)) + \cos(\pi\delta_l)\sin(\pi(\nu - l))\} \\ &= C(r)e^{r/\nu}\sin(\pi(\nu - l + \delta_l)) \end{aligned}$$

* 此时，因为有了core的影响，或者说，我们上面求的是在远处的行为，之后还会在与核里面的接起来，所以把g加上。
* （原来的波函数因为原点处不发散的条件，只保留了f这个方程的解）
然后我们再次要求无穷远处的波函数趋于0（作为边界条件）这样sin里面那一项需要为0。最后解出来，波函数是氢原子的波函数（即原来的波函数）产生了一个“相移”

$$\nu - l + \delta_l = n'$$

2. polarization

$$H = V_{pol}^{d}(r) + V_{pol}^{q}(r)$$

$$= -e^2 \frac{\vec{R}\cdot\vec{r}}{r^3} - \frac{1}{2}e^2 \frac{r}{r^3}\left[3\left(\frac{\vec{R}\cdot\vec{r}}{r}\right)^2 - R^2\right]$$

微扰 $$\sum_{m,p} \frac{|\langle \psi_{mq}|H|\psi_{mq}\rangle|^2}{E_0 - E_m - E_p} = \alpha - \frac{\alpha_d}{2r^4} - \frac{\alpha_q}{2r^6}$$

Rydberg原子之间的相互作用：偶极相互作用

$$V(\vec{R}) = \frac{1}{4\pi\varepsilon_0}\left\{\frac{\vec{\mu}_1\cdot\vec{\mu}_2}{R^3} - \frac{3(\vec{\mu}_1\cdot\vec{R})(\vec{\mu}_2\cdot\vec{R})}{R^5}\right\}$$

由于相互作用，能级发生移动。能级的移动大于线宽时，（Rydberg原子寿命比较长，所以线宽比较窄），造成Dipole Blockage，只能激发一个，不能两个原子都激发。

换句话说，第二个原子能否被激发，取决于第一个原子的状态。可以做成一个CNOT门。

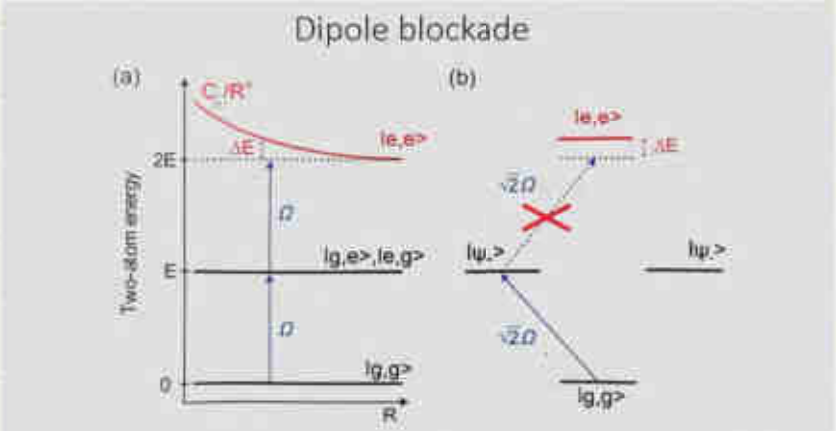


Figure 1.6: Pictorial representation of the dipole blockade principle. (a) Energy shift as a function of the interatomic distance. (b) Case when the dipole-dipole energy shift is larger than the transition linewidth. $|e,e\rangle$ denotes the double excited state, and $|\psi_+\rangle$ and $|\psi_-\rangle$ the symmetric and anti-symmetric states with one excitation only.

Chapter 6 Helium

多一个电子，成为He之后，Bohr的旧量子论就不能用了，必须用量子力学

$$P_{12}\psi(1,2) = \lambda\psi(1,2)$$

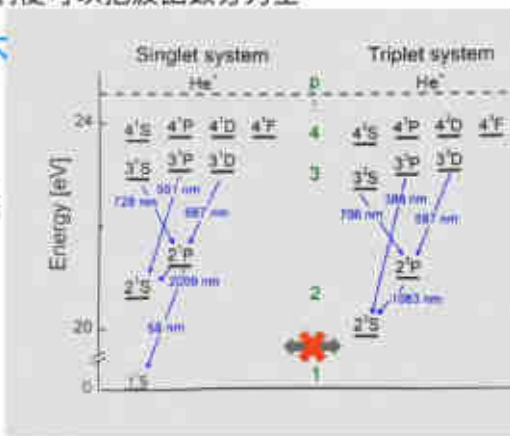
$$P_{12}^2\psi(1,2) = \lambda^2\psi(1,2)$$

$$\Rightarrow \begin{cases} \lambda = +1 & \text{para-state} \\ \lambda = -1 & \text{ortho-state} \end{cases}$$

10.1.2 正氦和仲氦（Orthohelium & Parahelium）

在考虑氢的粗能级结构（gross structure）的时候并不需要考虑到电子的自旋。但是，对于氦原子，我们一开始就需要考虑到自旋的作用。当考虑到自旋作用之后，我们便可以把波函数分为空间部分和自旋部分。

加磁场之后，两个态会一起转，也不能实现三重态和单重态之间的跃迁。



$$\psi = \psi_{space}\chi_{spin}$$

根据泡利不相容原理，该波函数必须是交换反对称的，因此有两种可能：

$$\psi = \psi^A_{space}\chi^S_{spin} \quad \text{or} \quad \psi^S_{space}\chi^A_{spin}$$

ortho, 正　　para, 仲

具体写来为：

$$\psi = \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)] \cdot \overset{\chi_A}{\boxed{\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}}, \qquad S = 0$$

Singlet System

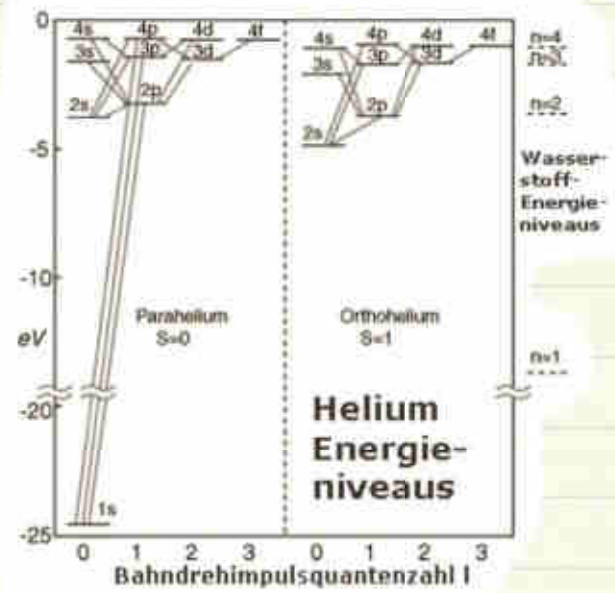
or

$$\psi = \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)] \cdot \boxed{\begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\downarrow\downarrow\rangle \end{cases}}, \qquad S = 1$$

χ_S

Triplet System, 无 1^3S

因此，我们把自旋为0的态叫做仲氦(parahelium)，自旋为1的态作为正氦(orthohelium)。在跃迁的时候，自旋不变。因为 $\langle\psi|\vec{r}|\psi\rangle$ 与自旋无关。所以，仲氦和正氦是两套跃迁系统：



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注意到，这里并没有 1^3S 态。Pauli也是据此得出Pauli不相容原理的。(因为两电子的空间波函数

氦是比氢多一个电子的原子，但是计算更为复杂（没有解析解）。它的哈密顿量为：

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\epsilon_0}(\frac{Z}{r_1} + \frac{Z}{r_2}) + \frac{e^2}{4\pi\epsilon_0}\frac{1}{r_{12}} - \frac{\hbar^2}{2M}(\nabla_1 \cdot \nabla_2)$$

这里取个近似。因为 $M \gg m$ 因此最后一项可以省略。此时，哈密顿量变为量三项，分别是动能项、核-电子库伦作用项 和 电子-电子库伦作用项。因为电子间的相互作用为斥力，因此也叫做排斥力项（repulsion term）。

在实验中我们可以得到氦的第一电离能和第二电离能，并据此可以计算出氦原子的基态能量。(单位 1eV = 96.485 kJ/mol)

$He \to He^+$ $He^+ \to He^{++}$ $He \to He^{++}$ 24.6 eV54.4 eV79 eV

因此，我们可以得到氦原子的基态能量为-79eV。但是，根据类氢原子的公式 $E = Z^2/2\,a.u.$ 这里的单位为Hartree原子单位制 $1a.u. = \hbar^2/m_e a_0^2 = 27.2eV$ 又因为有两个电子，因此不考虑电子-电子相互作用项时，能量为 $Z^2 a.u. = 108.8eV$ 显著地低于实验所测出来的基态能量。

微扰法

微扰法非常简单，我们认为相互作用项为微扰，即 $H = H_1 + H_2 + H'$ 。此时非微扰项的基态本征态是1s1s. 因此， $\psi_{100}(r_1) = R_{10}(r_1)Y_{00}(\theta,\phi)$. 两个电子的本征态为，$\psi(r_1, r_2) = \psi_{100}(r_1)\psi_{100}(r_2)$. 此时，一阶微扰近似为：

$$\Delta E^{(1)} = \int \psi^*(r_1, r_2) H' \psi(r_1, r_2)\, d^3r_1 d^3r_2$$

$$|\psi_A\rangle = \psi_{100}(1)\psi_{100}(2)\chi_A$$
$$= \frac{Z^3}{\pi}\exp[-Z(r_1+r_2)]\chi_A$$

$$\Rightarrow \quad \Delta E^{(1)} = \frac{Z^6}{\pi^2}\int \exp[-2Z(r_1+r_2)]\frac{1}{r_{12}}\, d\vec{r}_1 d\vec{r}_2$$

利用 $\begin{cases} \frac{1}{r_{12}} = \sum_{l=0}^{\infty}\frac{(r_<)^l}{(r_>)^{l+1}}P_l(\cos\theta) \\ P_l(\cos\theta) = \frac{4\pi}{2l+1}\sum_{m=-l}^{+l} Y_{lm}^*(\theta_1,\phi_1)Y_{lm}(\theta_2,\phi_2) \end{cases}$

然后把积分区域分成两半，一半是r1<r2，一半是r1>r2

$$\Rightarrow \quad \Delta E^{(1)} = Z^6\int_0^\infty dr_1\, r_1^2 \int_0^\infty dr_2\, r_2^2 \exp[-2Z(r_1+r_2)]\frac{1}{r_>}$$
$$= 16Z^6\int_0^\infty dr_1\, r_1^2 \exp[-2Zr_1]\left[\frac{1}{r_1}\int_0^{r_1} dr_2\, r_2^2 \exp(-2Zr_2) + \int_{r_1}^\infty dr_2\, r_2 \exp(-2Zr_1)\right]$$
$$= \frac{5}{8}Z \quad a.u. \qquad (1\,a.u. = 27eV)$$
$$\xrightarrow{Z=2,\ He} 34eV$$

$$\Rightarrow \quad E \approx E^{(0)} + E^{(1)} = -Z^2 + \frac{5}{8}Z$$

$\frac{\Delta E}{E} \propto \frac{1}{Z}$ 质子数变大，相对修正会变小。

通过计算可以得到：

$$\Delta E^{(1)} = \int \rho_1(r_1) V_{21}(r_1) d^3 r_1 + \int \rho_2(r_2) V_{12}(r_2) d^3 r_2$$

这里的 V_{21} 指的是电子2在 r1 处的电势。

$$V_{21} = \int_0^{r_1} dr_2\, r_2^2 \rho_2(r_2) \frac{e^2}{4\pi\epsilon_0 r_{12}}$$

对于超出 r1 的部分，对势能没有贡献。之所以这样做是因为我们需要分解 $1/r_{12}$：

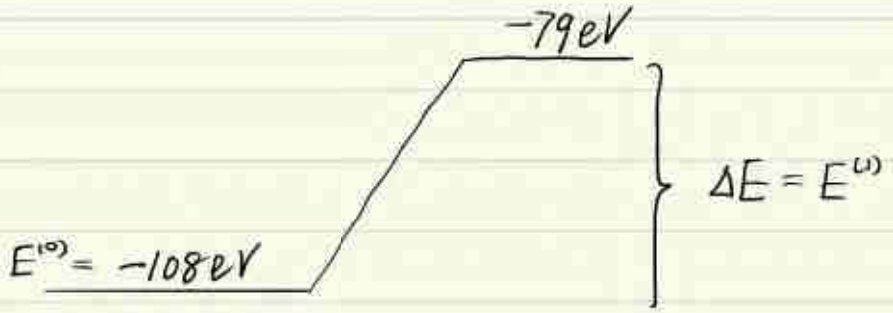
$$\begin{aligned}
\frac{1}{r_{12}} &= \frac{1}{r_2} \sum_{k=0}^{\infty} (\frac{r_1}{r_2})^k \frac{4\pi}{2k+1} \sum_{q=-k}^{k} Y_{k,q}^*(\theta_1, \phi_1) Y_{k,q}(\theta_2, \phi_2), \qquad k_2 > k_1 \\
&= \frac{1}{r_1} \sum_{k=0}^{\infty} (\frac{r_2}{r_1})^k \frac{4\pi}{2k+1} \sum_{q=-k}^{k} Y_{k,q}^*(\theta_1, \phi_1) Y_{k,q}(\theta_2, \phi_2), \qquad k_1 > k_2
\end{aligned}$$

$$\int Y_{k,q}(\theta_1, \phi_1) d\Omega = \delta_{q,0} \delta_{k,0}$$

因此，上述积分中只有k=0的球谐函数得以保留。用以方便计算，我们可以得到：

$$\Delta E^{(1)} = \frac{5}{8} Z\, a.u.$$

-108eV+34eV=79eV



He: Variational Method

变分法

变分法是一种求基态能量的方法。利用一个带参数的试探波函数去得到 $\langle\phi_c|H|\phi_c\rangle$. 我们认为在合适的参数c下得到的最小的能量就是基态能量。即：

$$\frac{\partial\langle\phi_c|H|\phi_c\rangle}{\partial c}=0$$

在这里，我们仍然采用1s1s态的波函数，参数为"核电荷数"Z。我们希望寻找更合适的Z。这里打引号是因为，我们并不改写哈密顿量，仅仅是让核电荷数为Z的波函数为试探波函数。

$$\phi_{trial}=\frac{Z^3}{\pi a_0^3}e^{-Z(r_1+r_2)/a_0}$$

在这样的波函数下，去把哈密顿量表达成如下的形式更易计算：

$$\begin{aligned}H=&-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)-\frac{e^2}{4\pi\epsilon_0}(\frac{Z}{r_1}+\frac{Z}{r_2}) && (H_0)\\&-\frac{e^2}{4\pi\epsilon_0}(\frac{Z-2}{r_1}+\frac{Z-2}{r_2}) && (H_1)\\&+\frac{e^2}{4\pi\epsilon_0}\frac{1}{r_{12}} && (V_{ee})\end{aligned}$$

根据类氢原子的公式，我们得到 $\langle\phi|H_0|\phi\rangle=-Z^2/2\,a.u.$ 对于第二项，我们计算得：

$$\begin{aligned}\langle\phi|H_1|\phi\rangle&=2\frac{e^2}{4\pi\epsilon_0}(Z-2)\langle\frac{1}{r}\rangle=2\frac{e^2}{4\pi\epsilon_0}(Z-2)\frac{Z}{a_0}\\&=2(Z-2)Z\,a.u.\end{aligned}$$

对于第三项和微扰项一致，因此为 $\langle\phi|V_{ee}|\phi\rangle=\frac{5}{8}Z\,a.u.$ 因此，我们可以得到一个总的能量为：

$$\begin{aligned}\langle H\rangle&=\langle H_0\rangle+\langle H_1\rangle+\langle V_{ee}\rangle\\&=-Z^2/2+2(Z-2)Z+\frac{5}{8}Z\quad a.u.\\&=Z(Z-\frac{27}{8})\quad a.u.\end{aligned}$$

当，$Z^*=\frac{27}{16}$ 时，上式具有最小值，$\langle H\rangle_{min}=-2.8477a.u.=-77.5eV$

这样子算出来更加接近实验值。

进阶的试探波函数 Hylleraas method

Hylleraas 提出了新的坐标系。他给出 $s=r_1+r_2$, $t=r_1-r_2$, $u=r_{12}$ ， 因此，哈密顿量中的势能部分（包括核与电子之间的库伦势）为：

本质上是一个"椭圆坐标系"。

$$V=-\frac{Z}{r_1}-\frac{Z}{r_2}+\frac{1}{r_{12}}=\frac{-4Zs}{s^2-t^2}+\frac{1}{u}$$

在这样的坐标下，他给出了如下形式的试探函数：

$$\phi(s,t,u)=e^{-ks}\sum_{l,m,n}^{N}C_{l,m,n}s^lt^{2m}u^n$$

当N=0，就是上面的结果。

这里的k为有效电荷数，N为这里考虑的项数，项数越多约精准。他得到的能量为 -2.90324 a.u. 与实验数值 -2.90372 在小数点后3位都一致。

10.1.4 激发态能量

所谓的激发态，就是一个电子是1s态，另一个电子是nl态（仍是按照类氢原子的态划分）。这里的激发态只考虑了单电子激发，因为，双电子激发的能量要大于氦离子的能量。因此，会出现俄歇效应Auger effect：

$$He^{**} \to He^{*} + e^{-}$$

而对于单电子激发态，能量不依赖于电子1或是2的标号，因此具有“交换兼并”(exchange degeneracy)的特性，所以，真实的波函数是这两个状态的线性组合。

$$\psi = a u_{1s}(1) u_{nl}(2) + b u_{1s}(2) u_{nl}(1)$$

仍然利用微扰法，我们得到，我们可以得到：

$$H'\psi = \Delta E \psi$$
$$\Leftrightarrow \begin{pmatrix} J & K \\ K & J \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \Delta E \begin{pmatrix} a \\ b \end{pmatrix}$$

direct integral $$J = \frac{e^2}{4\pi\epsilon_0} \int |u_{1s}(1)|^2 \frac{1}{r_{12}} |u_{1s}(2)|^2 d^3r_1 d^3r_2,$$ $$J = \frac{1}{2} \iint \frac{e^2}{r_{12}} \left\{ |\psi_{100}(1)|^2 |\psi_{nlm}(2)|^2 + (r_1 \leftrightarrow r_2) \right\}$$

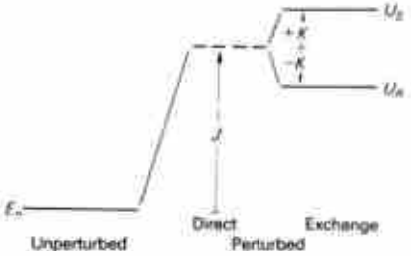
exchange integral $$K = \frac{e^2}{4\pi\epsilon_0} \int u_{1s}^*(1) u_{nl}^*(2) \frac{1}{r_{12}} u_{1s}(2) u_{nl}(1) d^3r_1 d^3r_2,$$ $$K = \frac{1}{2} \iint \frac{e^2}{r_{12}} \left\{ \psi_{100}^*(1) \psi_{nlm}^*(2) \psi_{100}(2) \psi_{nlm}(1) + (r_1 \leftrightarrow r \right.$$

因此，通过解这个方程，我们得到了对称和反对称的空间波函数。和微扰能量。它由直接积分和交换积分组成。

$$\left.\begin{aligned} \psi^A &= \frac{1}{\sqrt{2}}(u_{1s}(1)u_{nl}(2) - u_{1s}(2)u_{nl}(1)) \\ \psi^S &= \frac{1}{\sqrt{2}}(u_{1s}(1)u_{nl}(2) + u_{1s}(2)u_{nl}(1)) \end{aligned}\right\} \psi_\pm = \frac{1}{\sqrt{2}} \left\{ \psi_{100}(1)\psi_{nlm}(2) \pm \psi_{nlm}(1)\psi_{100}(2) \right\} \chi_{A/S}$$

$$\Delta E = J \pm K = J - \frac{K}{2}(1 + 4S_1 \cdot S_2)$$

$$\Delta E = \langle \psi_\pm | \frac{e^2}{r_{12}} | \psi_\pm \rangle = J \pm K \begin{cases} J+K, & \text{singlet} \\ J-K, & \text{triplet} \end{cases}$$



Energy levels of the excited-terms of the helium, shown is the effect of the direct integral J and the exchange integral K

avatar

态随时间变化

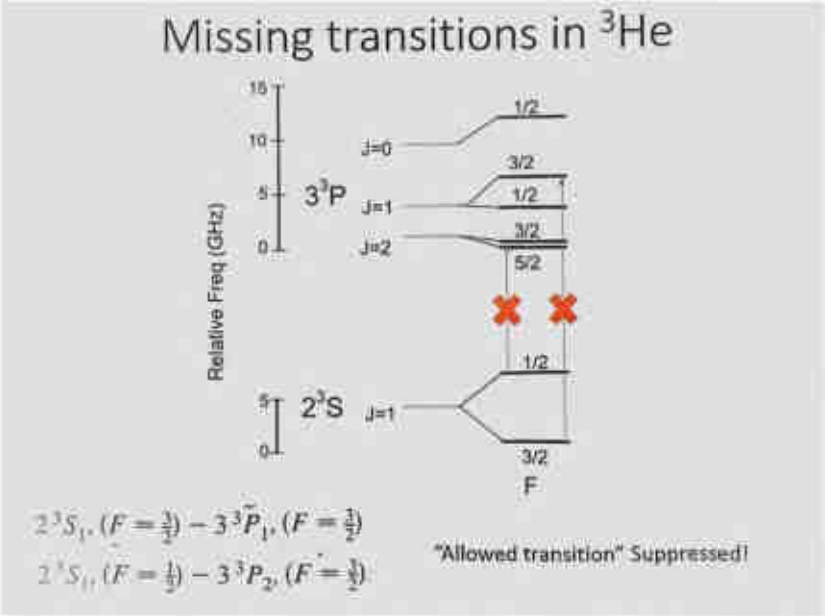
接下来我们考虑态在时间作用下会如何变化。我们不妨让初态设为：

$$\psi(t=0) = \psi_{100}(1)\psi_{nlm}(2) = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$

这里的正负态表达的是能量是J+K的态和J-K的态。因为他们的能量略有不同，因此，态的旋转的速率不同。 可以看出来叫交换积分的意义，两个态以交换能/hbar的频率进行交换。

$$\psi(t=T)=\frac{1}{\sqrt{2}}(\psi_+e^{i(J+K)T/\hbar}+\psi_-e^{i(J-K)T/\hbar})e^{iE_0t/\hbar}$$
$$=\frac{1}{\sqrt{2}}e^{-i(E_0+J)/\hbar}\{\psi_{100}(1)\psi_{nlm}(2)\cos(KT)-i\psi_{100}(2)\psi_{nlm}(1)\sin(KT)\}$$

所以当 $T=\pi/2K$ 的时候，两粒子态交换。K 是交换积分，与两粒子波函数的重叠面积有关。当两粒子比较近的时候，交换频率比较快。当激发到2s或2p态的时候， $T\sim10^{-14}s$ 而在比较远的态，比如 $l=9$ 的时候，时间甚至可以到 $T\sim1700years$.



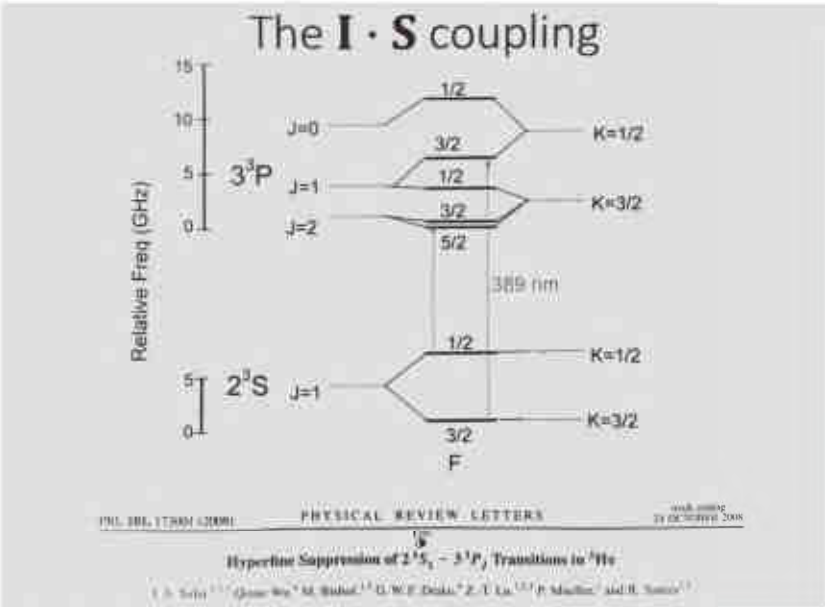
正常： $\vec{L}+\vec{S}\to\vec{J}$

$\vec{J}+\vec{I}\to\vec{F}$

选择定则本来在做角动量耦合的时候，有一些approximation的选择定则的项。左边这个在做微扰的时候，可以发现“微扰”的量级已经和原来的能级差比较接近了，这样的耦合方法不适用，应该换一种耦合方式：

现在： $\vec{S}+\vec{I}\to\vec{K}$

$\vec{K}+\vec{L}\to\vec{F}$



Hatree SCF（自洽场）

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{n}\nabla_i^2 - \sum_{i=1}^{n}\frac{Ze^2}{r} + \sum_{i\neq 1}^{n-1}\sum_{j=i+1}^{n}\frac{e^2}{r_{ij}}$$

0阶 $\phi^{(0)} = \prod_{i=1}^{n} S_i(r_i, \theta_i, \phi_i)$

$$S_1(r_1, \theta_1, \phi_1) = h_l(r)\, Y_{lm}(\theta, \varphi)$$

第一个电子看到其他电子对它形成的平均场：

$$V_{12} = \frac{e^2}{4\pi\varepsilon_0}\int \frac{|S_2|^2}{r_{12}} dv_2, \cdots, V_{1n} = \frac{e^2}{4\pi\varepsilon_0}\int \frac{|S_n|^2}{r_{1n}} dv_n$$

$$V_1(r_1, \theta_1, \phi_1) = V_{12} + \cdots + V_{1n} - \frac{Ze^2}{r_1 4\pi\varepsilon_0}$$

假设是球对称的，把上面的theta，phi积分积掉，得到 $V_1(r)$

$\Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + V_1(r)\right] S_1^{(1)}(r_1) = \varepsilon_1 S_1^{(1)}(r_1)$ ，都做一遍，得到一阶的：

1阶： $\phi^{(1)} = \prod_{i=1}^{n} S_i^{(1)}$

Chapter 7
Mathematical Method for Open System

7.1. Density Matrix

1. $\rho = \rho^{+}$
2. $Tr(\rho) = 1$
3. $\langle n|\rho|m\rangle \leq \langle n|\rho^2|m\rangle$
4. $\langle \hat{S}\rangle = Tr(\rho\hat{S})$

存在一个最大的可能的相干： $|\rho_{ij}|^2 < \rho_{ii}\rho_{jj}$

$$\rho = \begin{pmatrix} |c_1|^2 & c_1c_2^* \\ c_1^*c_2 & |c_2|^2 \end{pmatrix} \quad \text{(对纯态)}$$

n维的系统的最大混态（态与态之间完全没有相干）： $\hat{\rho} = \frac{1}{n}\hat{I}$

混态判据： $tr\rho^2 < 1$

混态对应Bloch球内的点，Bloch球中心对应最大混态。

基于密度矩阵，我们可以开始讨论开放体系：

系统的一组基矢是 $\{|s\rangle\}$，环境的一组基矢是 $\{|r\rangle\}$

两个空间的直积空间的基矢： $\{|s\rangle\otimes|r\rangle\}$

$$|\psi\rangle = \sum_{s,r}|s,r\rangle\langle s,r|\psi\rangle$$

$$\langle\hat{\sigma}\rangle = tr(\rho\hat{\sigma})$$

$$\Rightarrow \langle\hat{S}\rangle = \sum_{s,r}\langle s,r|\hat{S}|\psi\rangle\langle\psi|s,r\rangle$$

$$= \sum_s\langle s|\hat{S}\sum_r\langle r|\psi\rangle\langle\psi|r\rangle|s\rangle$$

$$= Tr_s(\hat{S}\hat{\rho}_s)$$

Partial trace： $\rho_s = Tr_R\,\rho$

分量形式：

$$\rho = \sum_{ij\mu\nu} C_{ij\mu\nu}|s_i\rangle\langle s_j|\otimes|r_\mu\rangle\langle r_\nu|$$

$$Tr_R\,\rho = \sum_{ij\mu\nu} C_{ij\mu\nu}|s_i\rangle\langle s_j|\langle r_\nu|r_\mu\rangle$$

7.2 System and environment

Since we are really only interested in the system, we would like to find a more e

In atomic physics and quantum optics, most environments are nearly Markovian, so we will focus on techniques for understanding the effects of a Markovian reservoir. So that the system is only influenced by the instantaneous state of the reservoir.

Again, we will assume $\hat{H} = \hat{H}_S + \hat{H}_R + \hat{H}_{SR}$. The interaction term $\hat{H}_S R$ is the most relevant part. To focus on it we will work in the interaction picture, which is found by transforming according to the unitary operator

$$\hat{U} = e^{i(\hat{H}_R + \hat{H}_S)t/\hbar}. \tag{3.37}$$

In the interaction picture (denoted by tildes), the relevant operators are

$$\tilde{\rho} = e^{i(\hat{H}_R+\hat{H}_S)t/\hbar}\hat{\rho}e^{-i(\hat{H}_R+\hat{H}_S)t/\hbar} \tag{3.38}$$

$$\tilde{H}_{SR} = e^{i(\hat{H}_R+\hat{H}_S)t/\hbar}\hat{H}_{SR}e^{-i(\hat{H}_R+\hat{H}_S)t/\hbar}. \tag{3.39}$$

这样,演化方程就只与相互作用 Hamiltonian 有关:

$$\frac{d}{dt}\tilde{\rho} = \frac{1}{i\hbar}[\tilde{H}_{SR}, \tilde{\rho}]$$

整体的演化: $\dot{\rho} = \frac{1}{i\hbar}[H, \rho]$, $H = \underbrace{H_S}_{\text{system}} + \underbrace{H_R}_{\text{reservoir}} + \underbrace{H_{SR}}_{\text{interaction}}$

$$\dot{\rho}_S = Tr_R(\dot{\rho}) = \underbrace{\frac{1}{i\hbar}[H_S, \rho_S]}_{\text{系统的相干演化}} + \frac{1}{i\hbar}Tr_R\{[H_R, \rho]\} + \underbrace{\frac{1}{i\hbar}Tr_R\{[H_{SR}, \rho]\}}_{\text{代表耗散}}$$

$Tr(AB) = Tr(BA)$, 这一项 $= 0$

Our analysis requires that the interaction be a bilinear product of system and reservoir operators:

$$H_{SR} = \hat{S}\hat{R}^{\dagger} + \hat{R}\hat{S}^{\dagger}$$

In the interaction picture, we will represent the Hamiltonian by

$$\tilde{H}_{SR} = \hat{S}\hat{F}_R^{\dagger}(t) + \hat{F}_R(t)\hat{S}^{\dagger}$$

For example, consider the Hamiltonian for a single atom interacting with the radiation field in the Schrodinger picture,

$H_{SR} = -\sum_j \hbar g_j \underbrace{a_j}_{\text{光子的湮灭算符}} |2\rangle\langle 1| + h.c.$

$$\hat{H}_{SR} = \underbrace{-\sum_j \hbar g_j \hat{a}_j}_{\hat{R}} \underbrace{|2\rangle\langle 1|}_{\hat{S}^{\dagger}} - \sum_j \hbar g_j^* \hat{a}_j^{\dagger} |1\rangle\langle 2|,$$

In addition to the specified form for the interaction, our analysis requires two assumptions regarding the nature of the reservoir itself, namely

(1) The reservoir is large (so it is not affected by the system)

(2) The reservoir has a broad bandwidth (so its correlation time is very short).

即相干时间 $\tau_c \sim \frac{1}{\text{bandwidth}}$ 很短

These assumptions together con- stitute the "Born-Markov Approximation", and a reservoir which satisfies them is called Markovian.

粗粒化处理，选一个做平均的时间尺度，在热库和系统的特征时间之间。

$$\tau_c < \Delta t < \tau_s$$

热库的相干时间　　系统演化的特征时间

经过一大堆推导：

做了粗粒化处理之后，例如对于二能级原子的辐射项，得到：

$$\frac{d\tilde{\rho}_s}{dt} = -\frac{\gamma}{2}\bar{n}(\omega)\left(\hat{S}\hat{S}^{+}\hat{\rho}_s - \hat{S}^{+}\hat{\rho}S\right) - \frac{\gamma}{2}(\bar{n}(\omega)+1)\left(\hat{S}^{+}\hat{S}\rho - \hat{S}\rho_s\hat{S}^{+}\right) + h.c.$$

其中 $\langle a_j^{+}\hat{a}_k\rangle = \delta_{jk}\bar{n}_j$

Master Equation　　$\frac{d\rho_s}{dt} = -\frac{i}{\hbar}[H,\rho_s] + \sum_j\left(2S_j\rho_s S_j^{+} + S_j^{+}S_j\rho_s + \rho_s S_j^{+}S_j\right)$

This result is known as the "master equation", and it provides an essential tool for studying the evolution of open systems coupled to Markovian reser- voirs. This formalism provides a method to properly treat non-unitary be- havior in the system of interest.

In the previous lecture we derived the equation governing the evolution of an open system coupled to a Markovian reservoir. In the Schrodinger picture, this so-called master equation takes the form

$$\begin{aligned}\frac{\Delta\hat{\rho}_S}{\Delta t} &= -\sum_p \frac{\gamma_p}{2}\bar{n}\left(\hat{S}_p\hat{S}_p^{\dagger}\hat{\rho}_S - \hat{S}_p^{\dagger}\hat{\rho}_S\hat{S}_p\right) + h.c. \\ &\quad -\sum_p \frac{\gamma_p}{2}(\bar{n}+1)\left(\hat{S}_p^{\dagger}\hat{S}_p\hat{\rho}_S - \hat{S}_p\hat{\rho}_S\hat{S}_p^{\dagger}\right) + h.c. \\ &\quad +\frac{1}{i\hbar}[\hat{H}_S,\hat{\rho}_S].\end{aligned}$$

1.3

The evolution of a driven two-level system coupled to a dissipative environmen

代入 $H_S = -\hbar\Delta|2\rangle\langle 2| + \hbar\Omega^*|1\rangle\langle 2| + \hbar\Omega|2\rangle\langle 1|$

令 $\hat{S} \equiv |1\rangle\langle 2| = \sigma_{12}$

where we have used $\hat{S} = |1\rangle\langle 2| = \sigma_{12}$ in Eq. (3.79), and $\sigma_{ij} = |i\rangle\langle j|$. Ta
the matrix elements $\langle i|\frac{\Delta\hat{\rho}_S}{\Delta t}|j\rangle = \dot{\rho}_{ij}$ yields four differential equations fo
components of the density matrix,

$$\begin{cases} \dot{\rho}_{22} = -\gamma(\bar{n}+1)\rho_{22} + \gamma\bar{n}\rho_{11} + i\Omega^*\rho_{21} - i\Omega\rho_{12} & (3 \\ \dot{\rho}_{11} = \gamma(\bar{n}+1)\rho_{22} - \gamma\bar{n}\rho_{11} - i\Omega^*\rho_{21} + i\Omega\rho_{12} & (3 \\ \dot{\rho}_{12} = -\frac{\gamma}{2}(2\bar{n}+1)\rho_{12} - i\delta\rho_{12} - i\Omega^*(\rho_{22} - \rho_{11}) & (3 \\ \dot{\rho}_{21} = -\frac{\gamma}{2}(2\bar{n}+1)\rho_{21} + i\delta\rho_{21} + i\Omega(\rho_{22} - \rho_{11}). & (3 \end{cases}$$

$$\begin{cases} \dot{\rho}_{11} = \gamma(\bar{n}+1)\rho_{22} - \gamma\bar{n}\rho_{11} - i\Omega^*\rho_{21} + i\Omega\rho_{12} \\ \dot{\rho}_{22} \\ \dot{\rho}_{12} = \boxed{-\frac{\gamma}{2}(2\bar{n}+1)\rho_{12}} - i\Delta\rho_{12} - i\Omega^*(\rho_{22} - \rho_{11}) \\ \rho_{21} = \rho_{12}^* \end{cases}$$

$-(\gamma_{12} + i\Delta)\rho_{12}$, $\bar{n} = 0$

$\dot{\rho}_{21} = -(\gamma_{21} - i\Delta)\rho_{21} + i\Omega(\rho_{22} - \rho_{11})$

$\gamma_{12} = \frac{\gamma_1 + \gamma_2}{2} + \gamma_{ph}$ 对角元的退相干只有一部分，导致布居数的改变。非对角元中既有gamma导致布居数改变，也有dephasing。

Three types of processes contribute to the system evolution described by Eq. (3.89):
(1) coherent driving Ω
(2) thermal photons $\gamma\bar{n}$, and
(3) spontaneous emission γ

Coherent interactions are characteristic of the ideal two-level system intro- duced in previous lectures, and come from the system Hamiltonian terms.

Thermal photons lead to incoherent transitions in both directions, whereas spontaneous emission only allows population in rho_22 to leak into rho_11.

Although incoherent processes can increase and decrease the populations ρ_{11} and ρ_{22}, they only decrease the off-diagonal terms. The decay rate of the coherences γ_{12} (defined through $\dot{\rho}_{12} = -\gamma_{12}\rho_{12} + \cdots$) is related to the rate of population decay out of state $|1\rangle$, $\gamma_1 = \gamma\bar{n}$, and $|2\rangle$, $\gamma_2 = \gamma(\bar{n}+1)$, by

$$\gamma_{12} = \frac{\gamma_1 + \gamma_2}{2} = \frac{2\bar{n}+1}{2}\gamma = \gamma_{21}. \tag{3.92}$$

While we see that there is a coherence decay rate associated with popu- lation decay, in general there also exist processes which decrease the coher- ences without a↔ecting the populations. These are typically incorporated phenomenologically into the master equation by setting:

$$\gamma_{12} = \gamma_{21} = \frac{\gamma_1 + \gamma_2}{2} + \gamma_d$$

dephasing rate

where γ_d is the so-called decoherence or dephasing rate. Such decoherence can result from a variety of sources including, for example, finite linewidth of an applied laser field or atom-atom interactions.

解方程（令 $\bar{n}=0$） 稳态解

（当 $\bar{n}=0$ 时， $\gamma_1=0$， $\gamma_2=\gamma$， $\gamma_{12}=\frac{\gamma}{2}$ $(+\gamma_d)$）

With this substitution, we find that in the weak field limit the coherence at frequency $\delta\nu$ is a Lorentzian with effective detuning $\delta+\delta\nu$:

$$\rho_{21}(\delta\nu)=\Omega(\delta\nu)\frac{i(\rho_{22}^{(0)}-\rho_{11}^{(0)})}{\gamma_{21}-i(\delta+\delta\nu)}.$$

This approach may be generalized to multilevel atoms, so that

$$\rho_{ij}(\delta\nu)=\Omega_{ij}(\delta\nu)\frac{i(\rho_{ii}^{(0)}-\rho_{jj}^{(0)})}{\gamma_{ij}-i(\delta_{ij}+\delta\nu)},$$

whenever the populations ρ_{ii} and ρ_{jj} are essentially frozen in time. For atoms approximately in the ground state ($\rho_{11}^{(0)}\approx 1, \rho_{22}^{(0)}\approx 0$), the atomic response resembles that of a classical dipole, as the atom acquires a dipole moment linear in the field strength. On the other hand, for sufficiently large Ω the quantized nature of the atom becomes important. In this case the population in the upper state cannot be neglected and leads to effects like non-linearity of the atomic response and saturation.

$$\dot{\rho}_{21}=0 \quad\Rightarrow\quad \rho_{21}=\frac{i\Omega(\rho_{22}-\rho_{11})}{\gamma_{21}-i\Delta}$$

$$+\ \dot{\rho}_{22}=0 \quad\Rightarrow\quad 0=-\gamma\rho_{22}+i\Omega^{*}\rho_{21}-i\Omega_{12} \qquad (\bar{n}=0)$$

$$\Rightarrow\quad \rho_{22}=\frac{R_{opt}}{\gamma+2R_{opt}}\to\frac{1}{2}.$$

$$\begin{cases} R_{opt}=2\gamma_{21}\dfrac{|\Omega|^2}{\gamma_{21}^2+\Delta^2}=2\gamma_{21}\dfrac{|\Omega|^2}{|\Gamma_{21}|^2} \\ \Gamma_{21}=\gamma_{21}-i\Delta \end{cases}$$

$$R_{opt}\ll\gamma \quad\Rightarrow\quad \rho_{22}\to 0$$
$$R_{opt}\gg\gamma \quad\Rightarrow\quad \rho_{22}\to\frac{1}{2}.$$

Ropt acts like an incoherent pumping rate associated with the applied (coherent) field.

In the first case, the coherent field is weak, so that the atom ends up in the ground state with almost unit probability. More specifically it can be seen that the population in the excited state is proportional to the field intensity in this limit $\rho_{22}\propto\Omega^2$ and the perturbative weak-field approach is valid. In the second case the applied field leaves the atom in a statistical mixture of the ground and excited states with equal weight, and the atomic response is said to be saturated.

Note that the weak-field limit is su

只要求 $|\Omega|^2 \ll \gamma_{21}^2 + \delta^2$

the populations change on a time scale much slower than the natural decay oscillation time of the coherence. The resulting equations for the populations

$$\dot{\rho}_{22} = -\gamma \rho_{22} + R_{opt}(\rho_{11} - \rho_{22}) \quad \text{with} \quad \dot{\rho}_{11} = -\dot{\rho}_{22}$$

Chapter 8

Propagation of Light in a Resonant Medium

8.1 Polarizability

之前我们研究的是光对原子的作用，现在再来研究原子对光的影响。

An atom influences the applied field through its dipole moment:

$$\langle \hat{d} \rangle = \mu \rho_{21} + \mu^* \rho_{12}$$

We neglect the interaction between the atoms, and think the atoms interact with light independently.

极化率 $$P = \frac{N}{V}(\mu\rho_{21} + \mu^*\rho_{12})$$

Self- consistency requires that this polarization then act as a source term in the Maxwell equations governing light propagation through the atomic cloud:

$$\begin{cases} \nabla \times \vec{E} = -\frac{\partial B}{\partial t} \\ \nabla \times \vec{B} = \frac{1}{c^2}\frac{\partial}{\partial t}\left(E + \frac{1}{\varepsilon_0}P\right) \end{cases}$$

In principle, we could now self-consistently calculate the evolution of the atomic medium and applied light field. In practice, we will typically deal with nearly monochromatic light fields, for which a considerable simplifica- tion can be obtained by using the slowly-varying envelope approximation.

在缓变包络近似下求解相互作用。先把Maxwell方程组写为：

$$\nabla^2 \vec{E} - \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = \frac{1}{\varepsilon_0 c^2}\frac{\partial^2 \vec{P}}{\partial t^2}$$

The wave equation is second order in time and space, but application of the slowly varying envelope approximation can reduce it to first order. An electric field which is nearly monochromatic can be parameterized by an envelope function and its central frequency ,

$$\begin{cases} \vec{E}(r,t) = \mathcal{E}(r,t)\, e^{ikz - i\omega t} + c.c. \\ \vec{P}(r,t) = P(r,t)\, e^{ikz - i\omega t} + c.c. \end{cases}$$

其中 $\mathcal{E}(r,t)$ 和 $P(r,t)$ 是缓变振幅。$\mathcal{E}$ (或P) 对参数 r,t 的依赖不敏感，相对 ω 及 $k=\frac{\omega}{c}$ 来说。

keeping only the lowest order derivatives of the envelopes, we find the evolution equation for the slowly varying amplitudes,

keeping only the lowest order derivatives of the envelopes, we find the evolution equation for the slowly varying amplitudes,

$$|\bar{\nu}\mathcal{P}| \;>>\; |\frac{\partial}{\partial t}\mathcal{P}|$$
$$|\bar{\nu}\mathcal{E}| \;>>\; |\frac{\partial}{\partial t}\mathcal{E}|$$
$$|\bar{k}\mathcal{E}| \;>>\; |\frac{\partial}{\partial z}\mathcal{E}|,$$

$$\nabla_\perp^2 \mathcal{E} + 2i\bar{k}\frac{\partial}{\partial z}\mathcal{E} + \frac{1}{c^2}2i\bar{\nu}\frac{\partial}{\partial t}\mathcal{E} = -\frac{1}{\epsilon_0 c^2}\bar{\nu}^2\mathcal{P},$$

or

$$\frac{1}{2i\bar{k}}\nabla_\perp^2 \mathcal{E} + \frac{\partial}{\partial z}\mathcal{E} + \frac{1}{c}\frac{\partial}{\partial t}\mathcal{E} = \frac{i\bar{k}}{2\epsilon_0}\mathcal{P}.$$

Two properties of this equation should be noted:

(1) In the first term, $\nabla_\perp^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ leads to transverse effects such as focussing or diffraction which cannot in general be neglected. However, for a plane wave there is no transverse spatial variation so the first term vanishes and we obtain

$$\frac{\partial}{\partial z}\mathcal{E} + \frac{1}{c}\frac{\partial}{\partial t}\mathcal{E} = \frac{i\bar{k}}{2\epsilon_0}\mathcal{P}.$$

(2) The slowly varying polarization $\mathcal{P}$ is proportional to the positive-frequency component of the dipole operator in the rotating frame. For example, a two level atom leads to a polarization $\mathcal{P} = (N/V)\mu\rho_{21}(z)e^{-i\bar{k}z}$. (Note that $\rho_{21}(z)$ itself is driven by the local electric field, which contains a fast phase term $e^{i\bar{k}z}$ so that $\mathcal{P}$ is in fact slowly varying in space.)

8.2 光传播的线性效应

光在介质中传播，场强非常弱，原子对它只有线性的响应。
在光与二能级原子相互作用的情况下：

$$P = \frac{N}{V}\mu \rho_{21} e^{ikz} = \varepsilon_0 \chi E$$

For plane wave propagation (where transverse effects may be disregarded), the SVEA equation reduces to

$$\frac{\partial \mathcal{E}}{\partial z} + \frac{1}{c}\frac{\partial \mathcal{E}}{\partial t} = \frac{i\bar{k}}{2\varepsilon_0} P$$

做一阶近似代入， $\frac{\partial \mathcal{E}}{\partial z} = \frac{i\omega}{c}\mathcal{E} + \frac{i\bar{k}}{2}\chi(\omega)\mathcal{E}$

解出$\mathcal{E}$对z的依赖： $\mathcal{E}(\omega, z) = \mathcal{E}(\omega, 0)\, e^{iz\left(\frac{\omega}{c} + \bar{k}\frac{\chi(\omega)}{2}\omega\right)}$

再代回原方程，得：

$$\mathcal{E}(t, z) = \int d\omega\, e^{-i\omega t}\, \mathcal{E}(\omega, 0)\, e^{iz\left(\frac{\omega}{c} + \bar{k}\frac{\chi(\omega)}{2}\omega\right)}$$

This solution tells us that, given the spectrum of the field at some position in space, we can decompose the field into frequency components, propagate each frequency component separately, and then transform back to the time domain to obtain the full solution. Note that we only need $\chi(\omega)$

(1) Absorption arises from the imaginary part of the susceptibility.

(2) Refraction is caused by the real part of the susceptibility.

(3) Dispersion results from frequency dependence of the susceptibility.

(1) 吸收与反射

共振时， $\mathcal{E}(\omega) \propto \delta(\omega)$，则 $\mathcal{E}(t, z) = \mathcal{E}\, e^{i\bar{k}\frac{\chi z}{2}}$ ， $\chi = \chi(0)$

$$\begin{cases} \alpha = \bar{k}\, \mathrm{Im}[\chi(0)] & \rightarrow \text{与振幅衰减有关} \\ n = 1 + \frac{\mathrm{Re}[\chi(0)]}{2} & \rightarrow \text{相位传播有关} \end{cases}$$

仍然要注意的是，我们这是在缓变包络近似之下得到的结果。

(2) 色散 (Dispersion)

If the applied field has a finite bandwidth, the frequency dependence of the susceptibility begins to matter. For nearly monochromatic fields, the susceptibility may be expanded around its resonant value, $\chi(\omega) \approx \chi(0) + \frac{d\chi}{d\omega}\omega + \cdots$

Each term leads to different effects: the first corresponds to refraction, the second to group velocity, the third to group velocity dispersion, and so on. For example, if we keep only the second order terms, we find

$$\begin{aligned}\mathcal{E}(t,z) &= \int d(\delta\nu)\mathcal{E}(\delta\nu,0)e^{-i\delta\nu t}e^{iz(\delta\nu/c+\bar{k}(\chi(0)+\frac{d\chi}{d\nu}\delta\nu)/2} \\ &= e^{iz\bar{k}\chi(0)/2}\int d(\delta\nu)\mathcal{E}(\delta\nu,0)e^{-i\delta\nu(t-z/v_g)} \\ &= e^{iz\bar{k}\chi(0)/2}\mathcal{E}(t-z/v_g, z=0),\end{aligned}$$

群速度： $v_g = \dfrac{c}{1+\frac{\bar{\omega}}{2}\frac{d\chi}{d\omega}}$

(3) 二能级系统

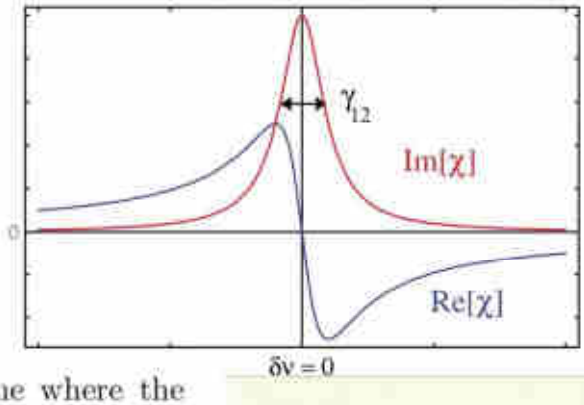
$$\chi(\omega) = i\frac{3}{8\pi^2}\frac{N}{V}\lambda^3(\rho_{11}-\rho_{22})\frac{\gamma}{\gamma_{12}-i\Delta}$$

$$\left(\ \chi(\delta\nu) = i\frac{N}{V}\frac{\mu^2}{\hbar\epsilon_0}(\rho_{11}^0-\rho_{22}^0)\frac{1}{\gamma_{12}-i\delta\nu}\ ,\ 且\ \gamma = \frac{\mu^2 k_0^3}{3\pi\epsilon_0\hbar},\ k_0 = \frac{2\pi}{\lambda}\ \right)$$

Lorentz Lineshape with Linewidth γ_{12}

spontaneous emission rate

We can plot the real (refractive) and imaginary (absorptive) parts of the susceptibility for a two-level atom near resonance



① **Resonant fields**

The magnitude of the susceptibility on resonance is

$$\chi(0) = i\frac{3}{8\pi^2}\frac{N}{V}\lambda^3\frac{\gamma}{\gamma_{12}}.$$

Here we have set $\rho_{11}^0 = 1, \rho_{22}^0 = 0$, since it is in the regime where the upper state is negligibly populated that the atom responds linearly to the field. Since $\chi(0)$ is purely imaginary, there is no refraction on resonance, but there is absorption. The electric field amplitude propagates as

$$\mathcal{E}(z) = \mathcal{E}(0)e^{(-\mathrm{Im}[\chi(0)]+i\mathrm{Re}[\chi(0)])\bar{k}z/2}$$

and we define the corresponding intensity loss

$$I(z) = I(0)e^{-N\bar{\sigma}z/V}$$

in terms of the absorption cross-section

均匀辐射展宽时，$\gamma = \gamma_{12}$

$$\begin{aligned}\bar{\sigma} &= \frac{3}{4\pi}\lambda^2\frac{\gamma}{\gamma_{12}} \\ &\to \frac{3}{2\pi}\lambda^2 \text{ for purely radiative broadening.}\end{aligned}$$

Unitary Limit

Surprisingly, in the case of radiative broadening the resonant cross section is independent of the atomic dipole moment and depends only on λ^2: this

② 大失谐情形

Far from resonance, $\delta\nu \gg \gamma_{12}$, the imaginary (absorptive) component $\mathrm{Im}[\chi] \propto 1/\delta\nu^2$ is much smaller than the real (reactive) component $\mathrm{Re}[\chi] \propto 1/\delta\nu$, so the medium is almost entirely refractive and causes little absorption.

(5) 谱线的展宽

The existence of the unitary limit shows that different line broadening mech- anisms (e.g. radiative vs non-radiative) can have different effects on the behavior of a system. It is particularly important to distinguish between processes which affects every atom equally and processes which broaden the linewidth of an ensemble but not its constituent atoms. The former "homo- geneous" linewidth may not be visible in an ensemble exhibiting the latter "inhomogenous" broadening. Two important examples of systems exhibit- ing inhomogeneous broadening are

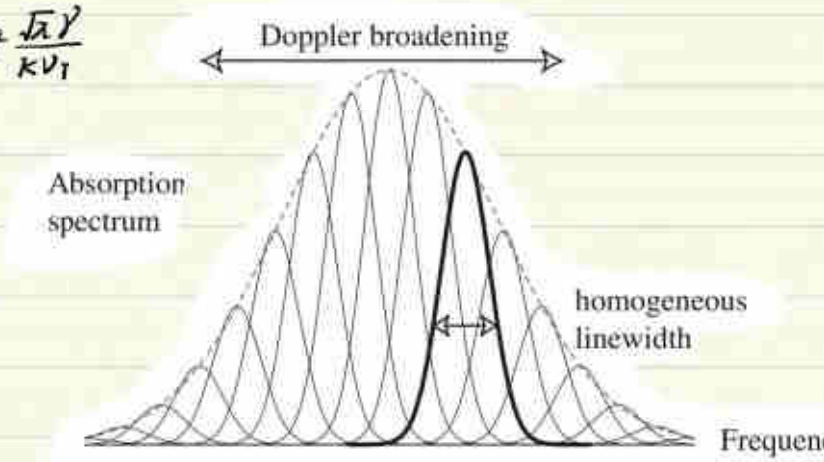
(1) Optical emitters (e.g. color centers or quantum dots) in a solid state environment. Local fields have a strong influence on the optical transitions, so each emitter will exhibit different transition strengths and frequencies.

(2) Atoms with a thermal velocity distribution. The Doppler effect shifts their resonant frequency, so each atom interacts differently with applied fields.

$$\chi(\omega) = \int dv_z \frac{n(v_z)}{\gamma_{12} - i(\omega - kv_z)}$$

$$n(v_z) = \frac{N}{V} e^{-\frac{v_z^2}{v_T^2}} \frac{1}{\sqrt{\pi}\, v_T}$$

$$\sigma_{inhom.}(0) = \frac{3}{4\pi}\lambda^2 \frac{\sqrt{\pi}\,\gamma}{k v_T}$$



8.3 原子对光的非线性响应

As a special case, we will consider only continuous-wave fields of fixed frequency, and look for the steady-state behavior of the system. To start with, consider a homogeneous ensemble of two-level atoms

Recall that the steady-state solution for the off-diagonal density matrix components is

$$\rho_{21} = -i\frac{\Omega}{\gamma_{12}-i\Delta}(\rho_{11}-\rho_{22})$$

For strong fields, we can no longer neglect changes in the atomic populations, so we should substitute (in the steady state)

$$\begin{cases} \rho_{11}-\rho_{22} = \dfrac{\gamma}{\gamma+2R_{opt}} \\ R_{opt} = \dfrac{2|\Omega|^2\gamma_{12}}{\gamma_{12}^2+\Delta^2} \end{cases}$$

We can use the steady state coherence to find the nonlinear susceptibility in the Fourier domain:

$$\chi_n(\Delta) = \frac{P(\Delta)}{\epsilon_0 \mathcal{E}(\Delta)} = \frac{1}{\epsilon_0 \mathcal{E}(\delta)}\frac{N}{V}\mu\rho_{21}(\Delta)$$

同理如前，得出：

$$\chi_n(\Delta) = \frac{3}{8\pi^2}\frac{N}{V}\lambda^3\frac{i\gamma}{\gamma_{12}-i\Delta}\frac{\gamma}{\gamma+2R_{opt}}$$

Note that, whereas the linear susceptiblity provided a complete solution to all time-dependent linearly propagating fields, the nonlinear susceptiblity only $\chi_n(\Delta)$ remaining terms are

$$\frac{\partial\mathcal{E}}{\partial z} = i\bar{k}\chi_n(\Delta)\mathcal{E} = i\bar{k}\left(\frac{3}{8\pi^2}\frac{N}{V}\lambda^3\frac{i\gamma}{\gamma_{12}-i\Delta}\frac{\gamma}{\gamma+2R_{opt}}\right)\mathcal{E}$$

这个 nonlinear susceptbility 与所加外场强度有关，$\Omega = \frac{\mu\mathcal{E}}{\hbar}$

当 $R_{opt} \ll \gamma$，就回到了上面线性情形

① **Resonant fields**

For a perfectly resonant field, $\delta = 0$, the real part of the susceptibility vanishes and the imaginary part becomes

$$\mathrm{Im}[\chi_n(0)] = \frac{3}{8\pi^2}\frac{N}{V}\lambda^3\frac{\gamma}{\gamma_{12}}\frac{1}{1+s}$$

吸收效应

where

$$s = \frac{4|\Omega|^2}{\gamma_{12}\gamma}.$$

→ Saturation parameter (in $\Delta=0$)

When this saturation parameter s is large, $s \gg 1$, the applied field bleaches the medium, and the transmitted power grows nonlinearly as the incident intensity is increased. In this saturated regime, the spatial profile of absorption changes qualitatively from a linear decay in strong fields to the

② 大失谐情形

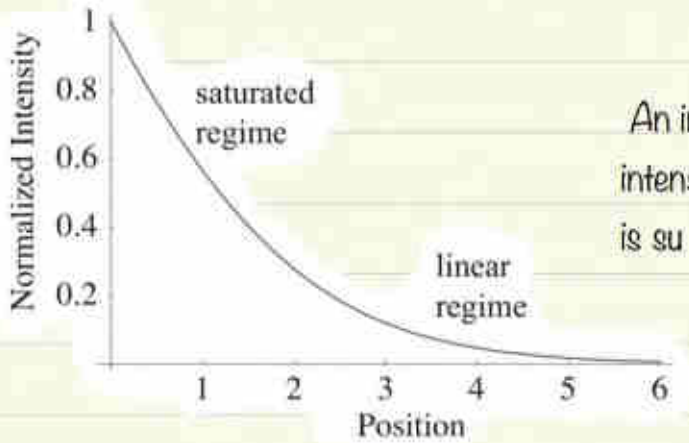
Re-define the saturation parameter:

$$S = \frac{2R_{opt}}{\gamma}, \qquad R_{opt} = \frac{2|\Omega|^2\gamma_{12}}{\gamma_{12}^2+\Delta^2}$$

当 very-large detuning, $\Delta \gg \Omega, \gamma$

The imaginary of χ is negligible, with the real part:

$$\chi_n \approx -\frac{3}{8\pi^2}\frac{N}{V}\lambda^3\frac{\gamma}{\Delta}\left(1-\frac{4|\Omega|^2\gamma_{12}}{\Delta^2\gamma}\right)$$



An incident field with intensity equal to the saturation intensity initially decays linearly with distance. Once the field is su

The physics of an intensity dependent refractive index (known as the Kerr effect) may be captured by defining an index which is linear in intensity, $n = n_0 + n_2 I$. Such effects have important physical consequences, including intensity-dependent phase shifts which are often referred to as "self-phase modulation". In addition, the medium will act as a lens for a beam with finite transverse extent, since the refractive index is a function of power and thus transverse position, leading to so-called self-focussing or de-focussing.

③ 弱饱和情形

试图计算对线性结构二阶近似，把 susceptibility 展开：

$$\begin{aligned}
\chi_n(\delta) &= \frac{3}{8\pi^2}\frac{N}{V}\lambda^3\frac{i\gamma}{\gamma_{12}-i\delta}\frac{\gamma}{\gamma+2R_{opt}} \\
&\approx \frac{3}{8\pi^2}\frac{N}{V}\lambda^3\frac{i\gamma}{\gamma_{12}-i\delta}\left(1-\frac{2R_{opt}}{\gamma}\right) \\
&\approx \underbrace{\frac{3}{8\pi^2}\frac{N}{V}\lambda^3\frac{i\gamma}{\gamma_{12}-i\delta}}_{\text{线性}} - \underbrace{\left(\frac{3\lambda^3}{2\pi^2\hbar^2}\frac{N}{V}\frac{i}{\gamma_{12}-i\delta}\frac{|\mu|^2\gamma_{12}}{\gamma_{12}^2+\delta^2}\right)|E|^2}_{\text{非线性}}
\end{aligned}$$

Chapter 9

Coherent Interaction in Multi-Level System

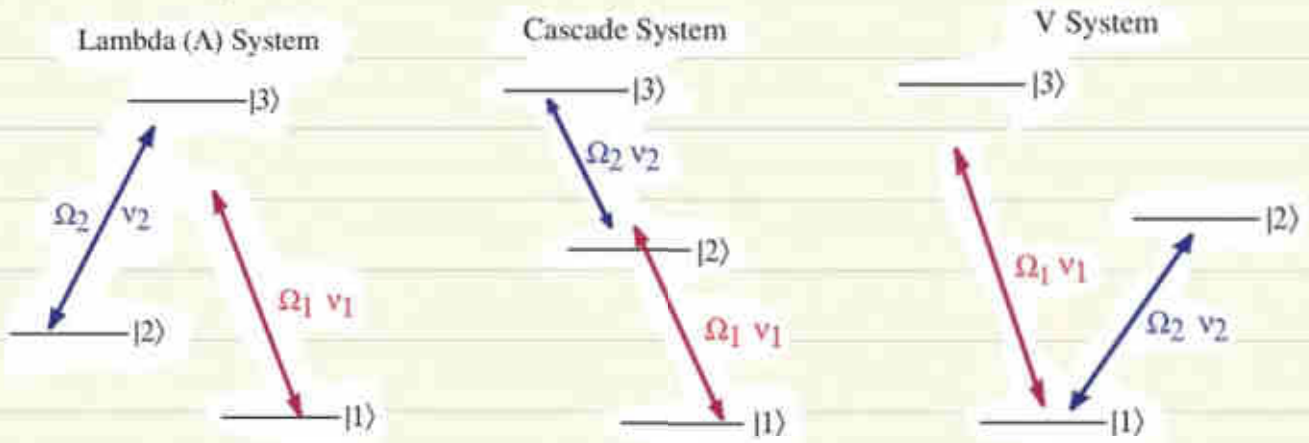
In previous lectures we have concentrated on understanding the interaction of a two-level atom with a single quasi-monochromatic beam of light. We now turn to multi-level systems which interact with multiple optical fields. Such multi-photon processes can be roughly organized into three classes:

(1) Incoherent interactions: Atomic coherences (e.g. off-diagonal ele- ments of the atomic reduced density matrix) are not important. One type of incoherent process which we have already seen is saturation spectroscopy, where one applied field modifies the atomic populations while the other field probes them.

(2) Coherent interactions: Atomic coherences are important, and two or more photons are required to generate them. A typical example of a coher- ent interaction is a Raman transition, where two photons can stimulate a dipole-forbidden transition via an excited state.

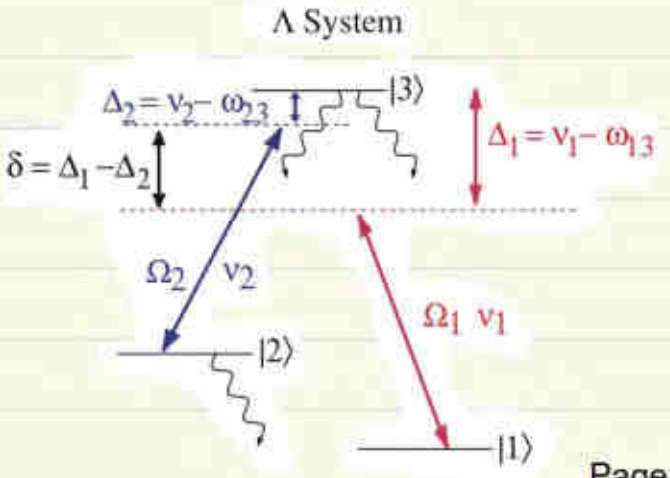
(3) Parametric interactions: No energy is exchanged between the light and the atoms, but the atoms mediate interactions between multiple light beams as in, for example, four-wave mixing.

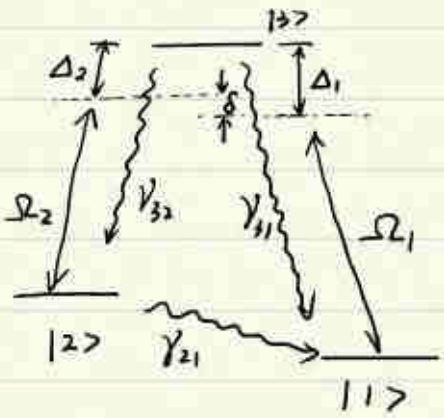
本章讨论第二种。



讨论V系统，其中 |2⟩与|1⟩之间是偶极禁戒的，

而 |1⟩和|3⟩、|2⟩和|3⟩是允许的。





9.1 The Schrodinger equation approach

一般光2比光1强很多，所以原子大部分处在1态上面。

已经去掉了快变项

$$\hat{H} = -\Delta_1 |3\rangle\langle 3| - \delta |2\rangle\langle 2| - \left(\Omega_1 |3\rangle\langle 1| + \Omega_2 |3\rangle\langle 2| + \Omega_1^* |1\rangle\langle 3| + \Omega_2^* |2\rangle\langle 3|\right)$$

$$|\psi\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle + c_3(t)|3\rangle$$

相当于换了一个相互作用绘景，在这个绘景下3的能量就对应于Delta_1

系数演化.

$$\begin{cases} \dot{c}_1 &= i\Omega_1^* c_3 \\ \dot{c}_2 &= i\delta c_2 + i\Omega_2^* c_3 \\ \dot{c}_3 &= i\Delta_1 c_3 + i\Omega_1 c_1 + i\Omega_2 c_2 \end{cases}$$

做这样一个近似，想把上面的态绝热地去除掉，认为c3上面的布居数很小

近似：大单光子失谐，(Large but similar single photon detuning)

$$\Delta_1 \sim \Delta_2 = \Delta \gg \Omega_1, \Omega_2, \gamma_3, \delta$$

与|3⟩的自然线宽有关

to lowest order in $\frac{\Omega_{1,2}}{\Delta}$, the excited state amplitude is constant:

$$c_3 = -\frac{\Omega_1 c_1 + \Omega_2 c_2}{\Delta}$$

substituting c_3 back to the equation:

$$\begin{cases} \dot{c}_1 &= -i\frac{|\Omega_1|^2}{\Delta}c_1 - i\frac{\Omega_2\Omega_1^*}{\Delta}c_2 \\ \dot{c}_2 &= i(\delta - \frac{|\Omega_2|^2}{\Delta})c_2 - i\frac{\Omega_1\Omega_2^*}{\Delta}c_1. \end{cases}$$

等效成二能级间的耦合，

$$\Omega_{eff} = -\frac{\Omega_2\Omega_1^*}{\Delta}$$

The effective two-level description is a good approximation.

By absorbing a photon on transition ω_1 and emitting a photon of frequency ω_2, population can be coherently transferred between the two ground states, leading to a large coherence $\rho_{21} = c_2 c_1^*$ Although we have neglected effects of the upper state decay, the excited state population is strongly suppressed by the large detuning Δ. Consequently, the probability for spontaneous emission is small, and the effective two-level description appears to be a good approximation.

In many situations, however, it will be necessary to account for the effects of dephasing and decay as well.

9.2 Density Matrix Approach

$$\dot{\rho} = \mathcal{L}_{31}(\rho) + \mathcal{L}_{32}(\rho) + i[\hat{H}, \rho],$$

where the Louvillian operators which account separately for decays from $|3\rangle$ to $|2\rangle$ and from $|3\rangle$ to $|1\rangle$ are given by e.g.

$$\mathcal{L}_{31} = -\frac{\gamma_{3\to1}}{2}\left(\sigma_{31}\sigma_{13}\rho - \sigma_{13}\rho\sigma_{31} + h.c.\right)$$

Using the Hamiltonian for the three-level system, we can find the coherent evolution of the density matrix components. The Louvillian operators will account for from $|3\rangle$ to $|1\rangle$ at rate γ, from $|3\rangle$ to $|2\rangle$ at rate $\bar{\gamma}$, and from $|2\rangle$ to $|1\rangle$ rate γ'. The total decay rate out of $|3\rangle$ is $\gamma_3 = \gamma + \bar{\gamma}$ whereas the total decay rate out of $|2\rangle$ is $\gamma_2 = \gamma'$. Finally, we will incorporate nonradiative decoherence mechanisms by setting the decay rate of a coherence ρ_{ij} to γ_{ij}. (In the limit of radiative decoherence γ_{ij} will be equal to half the sum of the decay rates out of $|i\rangle$ and $|j\rangle$.) The density matrix equations of motion for the lambda system are then

演化

$$\begin{cases} \dot{\rho_{11}} &= -i\Omega_1\rho_{13} + i\Omega_1^*\rho_{31} + \gamma\rho_{33} + \gamma'\rho_{22} \\ \dot{\rho_{22}} &= -i\Omega_2\rho_{23} + i\Omega_2^*\rho_{32} - \gamma'\rho_{22} + \bar{\gamma}\rho_{33} \\ \dot{\rho_{21}} &= -\left(\gamma_{12} - i\delta\right)\rho_{21} + i\Omega_2^*\rho_{31} - i\Omega_1\rho_{23} \\ \dot{\rho_{31}} &= -\left(\gamma_{13} - i\Delta\right)\rho_{31} + i\Omega_2\rho_{21} + i\Omega_1\left(\rho_{11} - \rho_{33}\right) \\ \dot{\rho_{32}} &= -\left(\gamma_{23} - i(\Delta - \delta)\right)\rho_{32} + i\Omega_2\left(\rho_{22} - \rho_{33}\right) + i\Omega_1\rho_{12} \end{cases}$$

where $\Delta = \Delta_1$. $\rho_{ij}^* = \rho_{ji}$, $\rho_{11} + \rho_{22} + \rho_{33} = 1$

Decay parameter:

$$\begin{cases} \Gamma_{12} &= \gamma_{12} - i\delta \\ \Gamma_{13} &= \gamma_{13} - i\Delta \\ \Gamma_{23} &= \gamma_{23} - i(\Delta - \delta) \end{cases}$$

9.3 5.1.3 The stochastic wavefunction method

The density matrix approach involves painful mathematics, but we can find a clever way around it by using the stochastic wavefunction method to incorporate decays without adding extra degrees of freedom. In particular, we will treat the system using a non-Hermitian Hamiltonian which adds two decay channels to the original Hermitian component,

$$\hat{H}_{\text{eff}} = \hat{H} - \frac{i\hbar\gamma_3}{2}|3\rangle\langle3| - \frac{i\hbar\gamma_2}{2}|2\rangle\langle2|.$$

有效哈密顿量.

We are free to use the Schrodinger equation $i\hbar|\psi\rangle = \hat{H}_{\text{eff}}|\psi\rangle$ so long as the probability for a quantum jump is small,

$$P_{\text{jump}} = \int dt\left(\gamma_2|c_2(t)|^2 + \gamma_3|c_3(t)|^2\right) \ll 1.$$

This constraint is satisfied in two important situations:

(1) If the system starts out in $|1\rangle$ and the probe field is weak, $\Omega_1 \to 0$, the populations in states $|2\rangle$ and $|3\rangle$ are of order $|\Omega_1|^2$ or higher, so to lowest order in Ω_1 we may neglect quantum jumps.

(2) If the system has finite population in both $|1\rangle$ and $|2\rangle$, quantum jumps are negligible provided that the decay from $|2\rangle$ is slow ($\gamma_2 \to 0$) and

上述 $\hat{H}_{eff}$ 可给出方程：

$$\begin{cases} \dot{c}_1 &= i\Omega_1^* c_3 \\ \dot{c}_2 &= -\underbrace{(\frac{\gamma_2}{2} - i\delta)}_{\Gamma_{12}} c_2 + i\Omega_2^* c_3 \\ \dot{c}_3 &= -\underbrace{(\frac{\gamma_3}{2} - i\Delta_1)}_{\Gamma_{13}} c_3 + i\Omega_1 c_1 + i\Omega_2 c_2 \end{cases}$$

解特殊情况的方程：

弱探测场 weak probe field Ω_1, constant field Ω_2 of arbitrary strength

$$\begin{cases} c_1(t) \approx 1 \\ \underbrace{(\frac{\gamma_2}{2} - i(\delta - \omega))}_{\Gamma_{12}} c_2 &= i\Omega_2^* c_3 \\ \underbrace{(\frac{\gamma_3}{2} - i(\Delta_1 - \omega))}_{\Gamma_{13}} c_3 &= i\Omega_1 + i\Omega_2 c_2 \end{cases}$$

(做了 Fourier 变化解方程)

解得：

$$\begin{cases} \rho_{11} = |c_1|^2 = 1 \\ \rho_{21} = c_1^* c_2 = -\dfrac{\Omega_1 \Omega_2^*}{\Gamma_{12}\Gamma_{13} + |\Omega_2|^2} \\ \rho_{31} = c_1^* c_3 = i\Omega_1 \dfrac{\Gamma_{12}}{\Gamma_{12}\Gamma_{13} + |\Omega_2|^2} \end{cases}$$

(其它的项都是小量可以忽略)

9.4 讨论 Large detuning Δ, weak Ω_1

When the probe is weak, we can characterize the response of the system by the linear susceptibility on the probe transition,

$$\chi_1 = \frac{|\mu|^2}{\hbar\epsilon_0}\frac{\rho_{31}}{\Omega_1},$$

which is proportional to

$$\begin{aligned} \frac{\rho_{31}}{\Omega_1} &= \frac{i}{\Gamma_{13}}\left(\frac{\Gamma_{12}}{\Gamma_{12} + |\Omega_2|^2/\Gamma_{13}}\right) \\ &= \frac{i}{\Gamma_{13}}\left(1 - \underbrace{\frac{|\Omega_2|^2/\Gamma_{13}}{\Gamma_{12} + |\Omega_2|^2/\Gamma_{13}}}_{\text{双光子跃迁的影响}}\right) \end{aligned}$$

|1⟩ 和 |3⟩ 之间对应的单光子跃迁

in the limit that $\Delta \gg \gamma_{13}$, 有 $\Gamma_{13} \approx -i\Delta$

$$\frac{|\Omega_2|^2}{\Gamma_{13}} = \frac{|\Omega_2|^2}{\gamma_{13} - i\Delta} \approx \frac{|\Omega_2|^2}{\Delta^2}(\gamma_{13} + i\Delta) \approx \frac{|\Omega_2|^2}{\Delta}$$

第二项变为：

$$\begin{aligned}
\frac{\rho_{31}}{\Omega_1} - \frac{i}{\Gamma_{13}} &\approx \frac{i|\Omega_2|^2/\Delta^2}{\Gamma_{12} + (|\Omega_2|^2/\Delta^2)(\gamma_{13} + i\Delta)} \\
&\approx \frac{i|\Omega_2|^2/\Delta^2}{\underbrace{(\gamma_{12}/2) + (\gamma_{13}/2)(|\Omega_2|^2/\Delta^2)}_{\gamma_{\rm eff}} - i\underbrace{(\delta - |\Omega_2|^2/\Delta)}_{\delta'}}
\end{aligned}$$

The real and complex parts of the denominator correspond to the effective width and detuning of the two-photon resonance. Because we have included decay, the susceptibility remains finite even on resonance.

做实验的时候，一般Omega2是固定的，然后扫Omega1

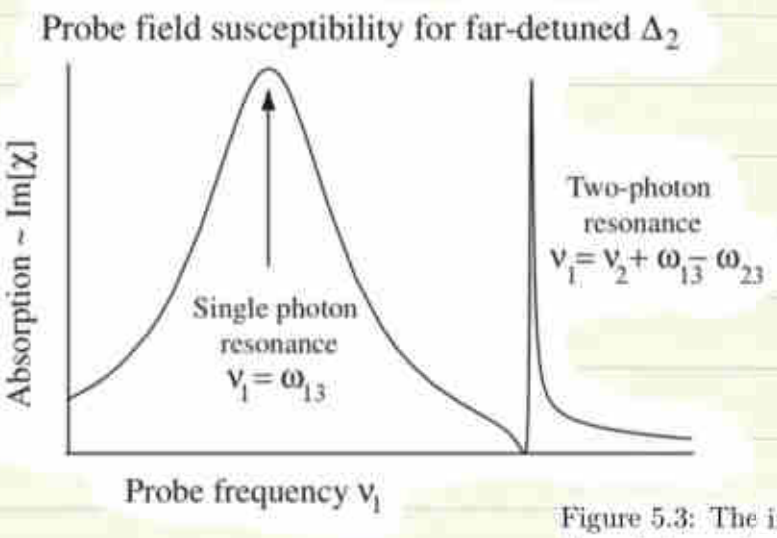


Figure 5.3: The imaginary part of the probe beam susceptibility as a function of the probe beam detuning. The absorption of Ω_1 exhibits a double resonance lineshape in the presence of a far-off resonant coupling beam Ω_2. In this calculation, $\gamma_{12} = 0$, so the single-photon and two-photon resonances have the same peak value, but the linewidth of the two-photon peak is significantly narrower.

Dressed state interpretation

We can obtain insight into the physical origin of this result by examining the system in the dressed state picture.

$$\begin{aligned}
|+\rangle &\approx |3\rangle - \frac{\Omega_2^*}{\Delta}|2\rangle \\
|-\rangle &\approx |2\rangle + \frac{\Omega_2}{\Delta}|3\rangle
\end{aligned}$$

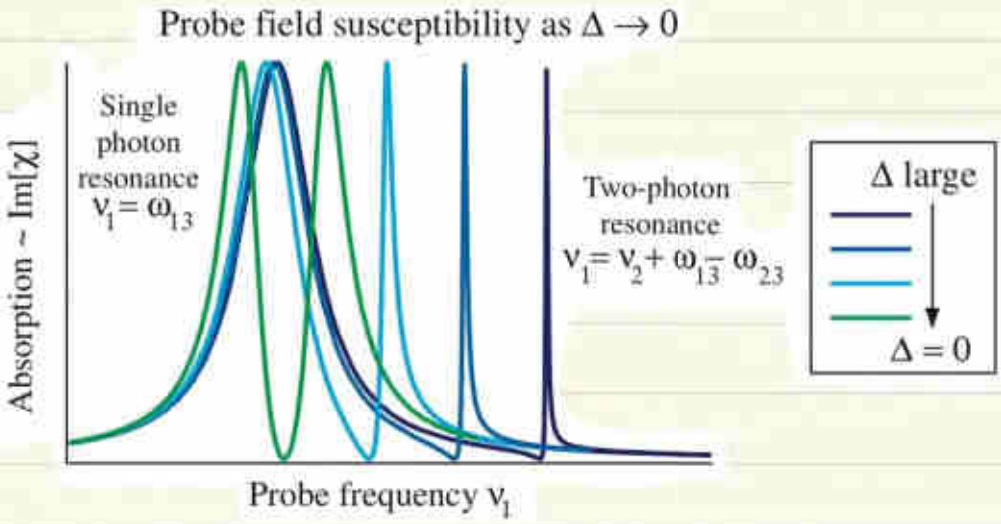
9.5 Resonant excitation: Electromagnetically induced transparency

The dark resonance

Consider an experiment where we illuminate the three-level atom with an applied field Ω_2 which is precisely on resonance, $\Delta_2 = 0$. We then sweep the frequency of the probe beam $\Delta_1 = \delta$, and observe how the susceptibility changes as a function of Δ_1. Using the expression we previously derived for the optical coherence on the ν_1 transition,

$$\boxed{\frac{\rho_{31}}{\Omega_1} = \frac{i}{\Gamma_{13}}\left(1 - \frac{|\Omega_2|^2/\Gamma_{13}}{\Gamma_{12} + |\Omega_2|^2/\Gamma_{13}}\right)}$$

保持 Ω_2 不变，$\Delta_2 = 0$，
扫描 probe light Δ_1
(即扫 δ 1)



当 $\delta = 0$ 时，absorption $= 0$，变成完全透明.

$$\begin{cases} \text{for } \Omega_2 \ll \gamma_{13}, \text{ the width of this absorption dip: } & \gamma_{12} + \frac{|\Omega_2|^2}{\gamma_{13}} \\ \text{for } \Omega_2 \gg \gamma_{13}, & \gamma_{12} + |\Omega_2| \end{cases}$$

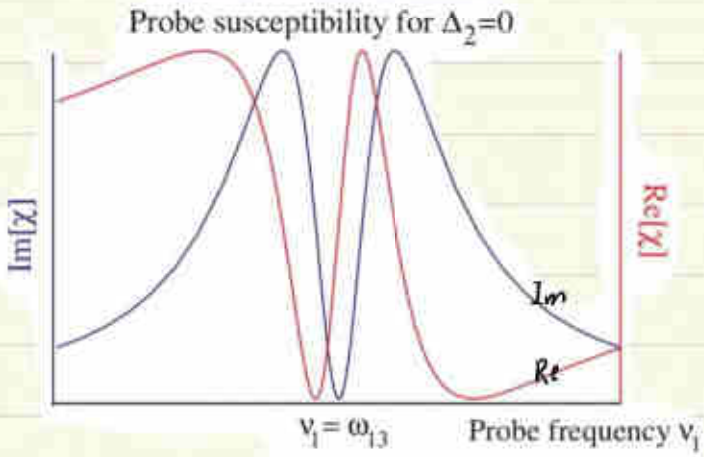


Figure 5.5: The real and imaginary part of the probe beam susceptibility are shown under resonant illumination by Ω_2. The absorption dip at zero detuning is known as a dark resonance or electromagnetically induced transparency.

共振的时候反而没有吸收了，完全透明。

双光子失谐为0的时候

To gain further intuition for the physics behind the dark resonance, we shall examine the non-Hermitian effective Hamiltonian. If the metastable decoherence rate vanishes, $\gamma_{12} = 0$, and the applied fields are precisely on resonance, $\Delta = \delta = 0$, the effective Hamiltonian becomes

此时不包含有耗散的作用。
不含有退相干的效应。

$$\begin{aligned}\hat{H}_{\text{eff}} &= -\frac{i\hbar\gamma_3}{2}|3\rangle\langle 3| - (\Omega_1^*|1\rangle\langle 3| + \Omega_2^*|2\rangle\langle 3| + h.c.) \\ &= -\frac{i\hbar\gamma_3}{2}|3\rangle\langle 3| - \underbrace{(\Omega_1^*|1\rangle + \Omega_2^*|2\rangle)}_{|B\rangle}\langle 3| - |3\rangle\underbrace{(\Omega_1\langle 1| + \Omega_2\langle 2|)}_{\langle B|}\end{aligned}$$

Note that the excited state $|3\rangle$ only couples to a particular superposition of the lower states, $|B\rangle$

the excited state and thus insensitive to its decay. This so-called dark state,

$$|D\rangle = \frac{\Omega_2|1\rangle - \Omega_1|2\rangle}{\sqrt{|\Omega_1|^2 + |\Omega_2|^2}}$$

is an eigenstate of the effective Hamiltonian with zero energy:

不与它耦合

$$\hat{H}_{\text{eff}}|D\rangle = 0.$$

A system in state $|D\rangle$ has vanishing absorption and polarization on the $|1\rangle$ to $|3\rangle$ transition, but finite polarization on the forbidden transition. Quantitatively, the density matrix for the dark state,

$$\rho = |D\rangle\langle D|,$$

完全是因为相干引起的，量子的效

has off-diagonal elements

$$\rho_{21} = -\frac{\Omega_2^*\Omega_1}{|\Omega_1|^2 + |\Omega_2|^2}.$$

In the limit that $\Omega_1 \ll \Omega_2$, we reproduce our previous result. Consequently, we see that the vanishing absorption on resonance is associated with the production of dark states which are decoupled from both light beams. This can also be viewed as a quantum interference phenomenon, where simultaneous excitations of $|3\rangle$ by Ω_1 and Ω_2 destructively interfere, leaving the excited state unpopulated by the applied fields.

Dispersive properties of the dark resonance: "slow light"

Thus far we have considered only the imaginary part of the probe susceptibility in the vicinity of the dark resonance. The real part leads to dispersive effects, since for $\Delta_2 = 0$ and δ small

$$\mathrm{Re}[\chi] \propto \mathrm{Re}[\frac{\rho_{31}}{\Omega_1}] \approx \frac{\delta}{|\Omega_2|^2 + \gamma_{12}\gamma_{13}}$$

In the situation relevant to the dark resonance, the slope of the refractive index $n \propto \mathrm{Re}[\chi]$ can be controlled by changing the intensity of Ω_2. In particular, this slope determines the group velocity since

$$v_g = \frac{d\omega}{dk} = \frac{c}{n(\omega) + \omega\frac{dn}{d\omega}}$$

越共振,群速度越小,趋向0.

(where $n(\omega)$ is the index of refraction) and $n(\omega) = 1 + \mathrm{Re}[\chi]/2$. The slope $\frac{dn}{d\omega}$ diverges as $\gamma_{12} \to 0$ and $\Omega_2 \to 0$:

$$v_g \approx \frac{c}{1 + \frac{\gamma_{13}\bar{\nu}3\pi(N/V)(\lambda/2\pi)^3}{|\Omega_2|^2+\gamma_{13}\gamma_{12}}}$$

so that the group velocity is reduced to zero as $\Omega_2 \to 0$ (see problem set 3 for a derivation of this formula). Simultaneously, the width Δw of the the resonance also vanishes, since

$$\Delta w \approx \frac{|\Omega_2|^2}{\gamma_{13}} \to 0$$

Note that when the linewidth is dynamically reduced while a pulse is travel- ling through the medium, careful considerations show that the spectrum of the pulse itself is also dynamically reduced. In particular, if the pulse spec- trum fits inside the transparency window initially, it fits in the window at a times and no dissipation is taking place (see problem set 3 and references therein for further details).

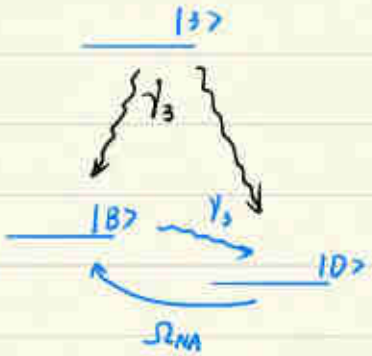
Since the two-photon resonance can be much narrower than the single-photon linewidth, the group velocity of the probe pulse Ω_1 can be reduced substantially below the speed of light. As resonant probe light enters the medium it compresses by a factor v_g/c, then slowly propagates through the atomic cloud, dragging along a spin coherence associated with the dark state. Since absorption vanishes, virtually all of the probe light is transmitted, with a significant delay due to the slow group velocity. This phenomenon is known as "electro-magnetically induced transparency" or "slow light".

9.6 Stimulated Raman Adiabatic Passage

绝热演化过程，最开始态在1上，通过对Omega
和Omega_2的调节，慢慢态转移到2上面。

Our discussion has not explained how the system is prepared in the dark state. In fact, if the probe light turns on slowly enough, the system will adiabatically follow from the initial state $|1\rangle$ to $|D\rangle$, in essence preparing itself. This phenomenon is an example of stimulated Raman adiabatic passage (STIRAP), whereby slowly varying applied fields can be used to eh are exquisitely sensitive to pulse amplitude and timing, STIRAP techniques do not depend on the details of pulse shape.

$$|\psi(t)\rangle = C_B(t)|B\rangle + C_3(t)|3\rangle$$



Ω_{NA} 要小，代表非绝热的影响，γ_3 要大

$$i\hbar \langle B|\frac{d}{dt}|D\rangle = i\hbar\frac{1}{\tau}$$

$$\begin{cases} \dot{C}_3(t) = -\gamma C_3(t) + i\Omega C_B(t) \\ \dot{C}_B(t) = i\Omega^* C_3(t) \end{cases}$$

$$\dot{C}_3 = 0 \Rightarrow C_3 = \frac{i\Omega}{\gamma} C_B$$

$$\Rightarrow \dot{C}_B(t) = -\underbrace{\boxed{\frac{\Omega^2}{\gamma_3}}}_{\gamma_B} C_B(t)$$

$$\Omega_{NA} \equiv \frac{1}{\tau}$$

绝热条件 $\frac{1}{\tau} \ll \gamma_B = \frac{|\Omega|^2}{\gamma_3}$

Under different applied powers:

$$\Omega_2 \to 0,\ \Omega_1 \text{ fixed} \Rightarrow |D\rangle = -|2\rangle$$

$$\Omega_1 \to 0,\ \Omega_2 \text{ fixed} \Rightarrow |D\rangle = |1\rangle$$

The physics here is fairly obvious, since $|1\rangle$ does not couple to Ω_2 and vice versa. Consequently, if the system starts out in the state $|1\rangle$ illuminated only by Ω_2, it is already in the dark state. By slowly decreasing Ω_2 while increasing Ω_1, the atomic state will adiabatically follow the dark state, finally ending up in $|2\rangle$ when $\Omega_2 = 0$. Since the dark state contains no component of the excited state, and does not couple to the light, the atomic state will be free from dissipation or decoherence from the excited state. Such manipulation is known as a "counter-intuitive pulse sequence," since the light is initially applied on the transition which is unpopulated.

Chapter 10 Doppler-free Spectroscopy

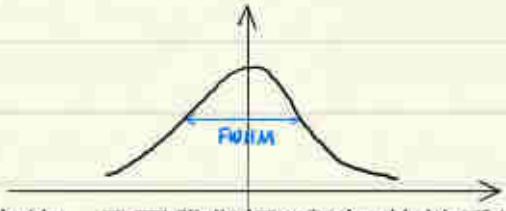
光和微波与原子的相互作用，理论上差不多，但是自发辐射的速率不同。
根据不同的特征时间，有时候用Bloch Equation，有时候用Optical Bloch Equation。

$$n_e = \frac{1}{2}\frac{1}{1+\frac{I_s}{I}\left(1+4\frac{\Delta^2}{\Gamma^2}\right)} \propto \frac{I/I_s}{1+\frac{I}{I_s}+4\frac{\Delta^2}{\Gamma}} \propto \frac{1}{1+4\frac{\Delta^2}{(1+\frac{I}{I_s})\Gamma^2}}$$

但是这是稳态的解，做了relaxation之后。

如果时间足够快，在relaxation之前，就有可能实现population inversion。

从上面公式可以求出来FWHM $= \sqrt{1+\frac{I}{I_s}}\,\Gamma$

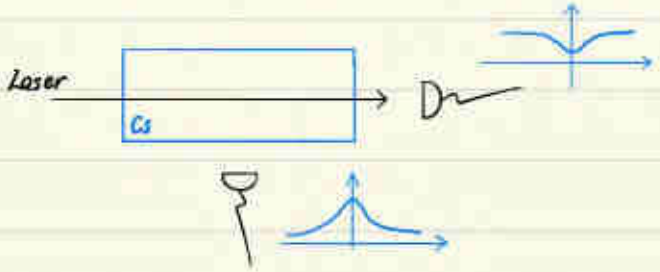


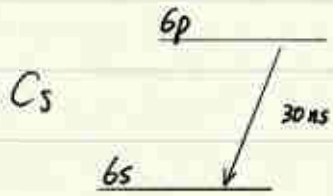
Γ是原子驰豫速率，$\Gamma = \frac{1}{\tau}$ 。$n_e(t) = n_0 e^{-\Gamma t} = n_0 e^{-\frac{t}{\tau}}$

Γ：自然线宽，natural linewidth　　由真空涨落的性质决定的。只要我们把“真空”的性质发生改变，就可以调节Gamma的大小。（Cavity QED）

加电场后，FWHM：$\Gamma \to \sqrt{1+\frac{I}{I_s}}\,\Gamma$，称 Power broadening，线宽会变宽。

光强变小之后虽然线宽比较窄，但是信号也会变小。需要找到一个平衡。





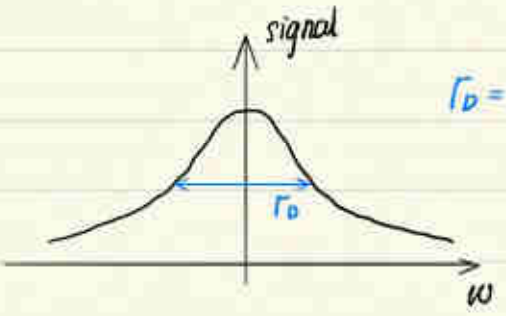
$\Gamma = 2\pi \cdot 6\,MHz$

调节激光的频率，可以看到这条光的线一会儿亮一会儿暗。

Doppler Broadening

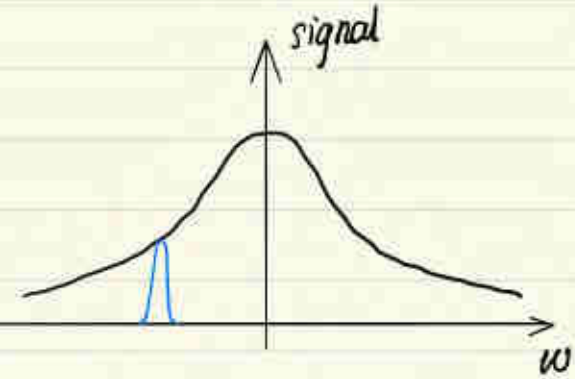
Maxwell distribution in 1D:　$p(v)dv \propto e^{-(\frac{v}{u})^2}dv$，$u = \sqrt{\frac{2k_BT}{m}} \approx 200\ m/s$

多普勒频移 $\Delta\omega_D = \omega_0\frac{u}{c} = kv = \frac{2\pi}{\lambda}v$　　量级是 $2\pi\times\frac{1}{4}\times10^8\,Hz$，几百 MHz 频率



$\Gamma_D = 2\sqrt{\ln 2}\,\omega_0\frac{u}{c} = 2\pi\cdot 390\ MHz$

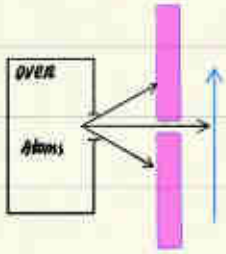
实际的表达式是所有的convolution。



一个特定频率的光，只能激发一个速度群的原子，这个速度群演着激光的方向的速度都是很相似的。（这是由于失谐不大的时候才能激发，而失谐是和Gamma比较，Gamma远小于Gamma_D，所以表现在图里面是蓝色的那一个小窄范围。

Doppler-free Spectroscopy

第一个简单的 Doppler-free方法：

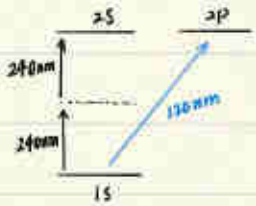


只让速度方向和激光垂直的原子通过，这样就没有一阶多普勒效应。

真正的共振：$\hbar\omega = \hbar\omega_0 + \left(\frac{\hbar k}{2m}\right)^2$

光打到原子上之后，原子存在反冲运动。例如测量同位素的不同时就要考虑。

第二个双光子跃迁的方法：



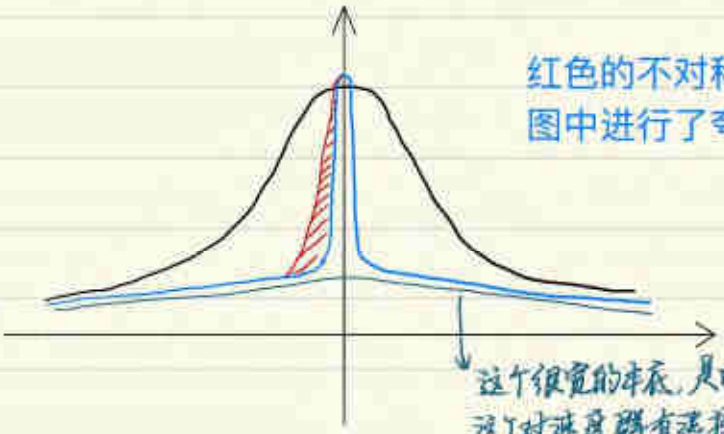
$\lambda < 200\,nm$ 真空紫外 VUV，Vaccum Ultra-violet

Two-Photon Transition Condition: $\Delta\omega = \omega_1 + \omega_2$

$\Delta\omega_D = \pm\omega_0 \frac{v}{c}$ 这样就不存在一阶多普勒频移。

（这个情形，原子也没有反冲）

Two-photon Spectroscopy：（蓝色的）



红色的不对称部分，是二阶多普勒效应的影响，图中进行了夸大。

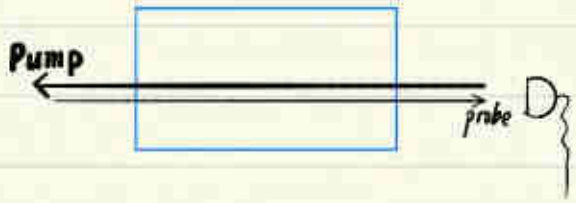
这个很宽的本底，是吸收了两个同向的光子。
这个对速度群有选择性，所以比较弱
velocity group

原子的光谱，自然线宽是洛伦兹线型$\propto \frac{1}{1+(\frac{\Delta}{\Gamma})^2}$

多普勒展宽是Gauss线型:$\propto e^{-(\frac{\Delta}{\sigma})^2}$

所以在很远的地方，事实上是洛伦兹线型占主要地位。

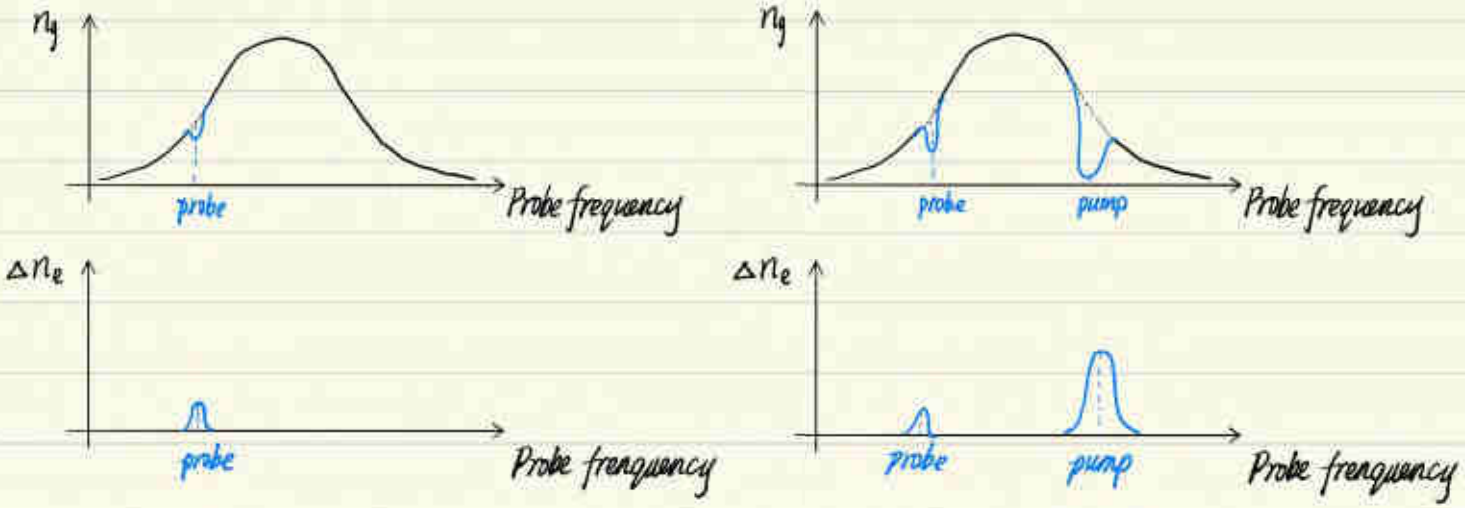
Saturation Absorption Spectroscopy:



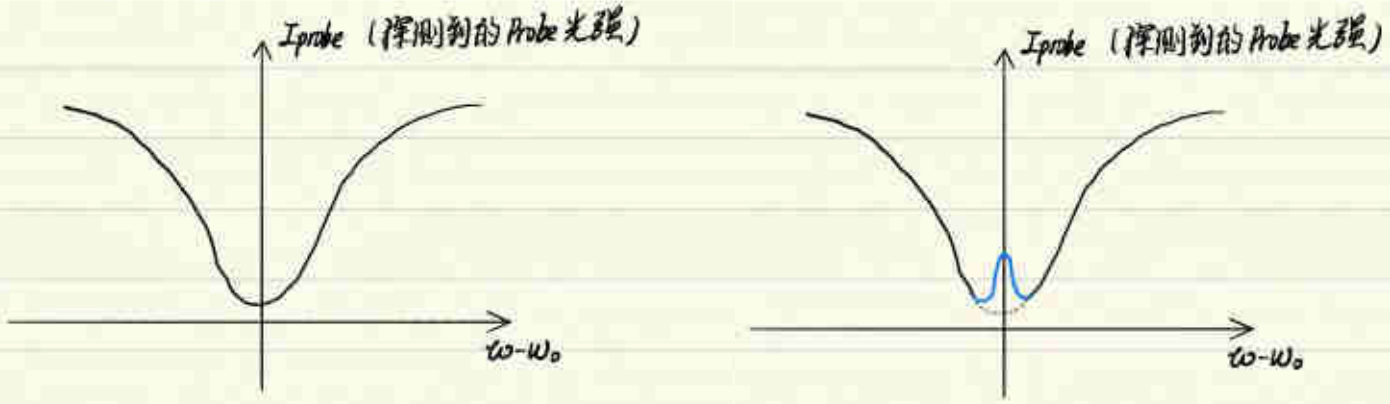
$I_{pump} > I_s$，很强

$I_{probe} < I_s$，较弱

(这两个光重合)



虽然Pump光和Probe光在空间上（坐标空间上）是重合的，但是在不在共振时，发生作用的原子的速度群不同。在共振时，激发的就是同一群原子。



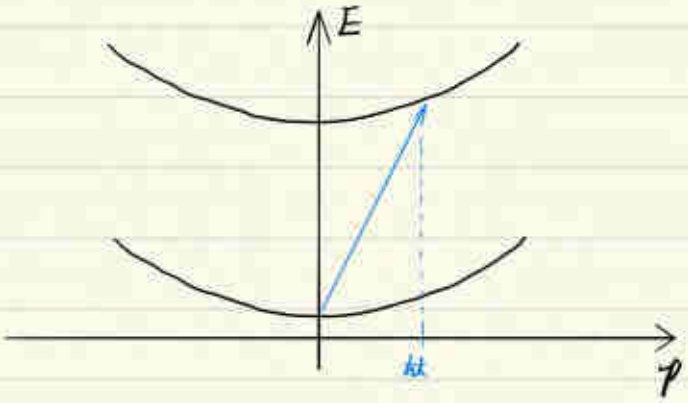
在共振时，他们相互作用的是同一群原子，就会发生“争夺”，产生Saturation。由于Pump光的强度很大于Probe光的强度，

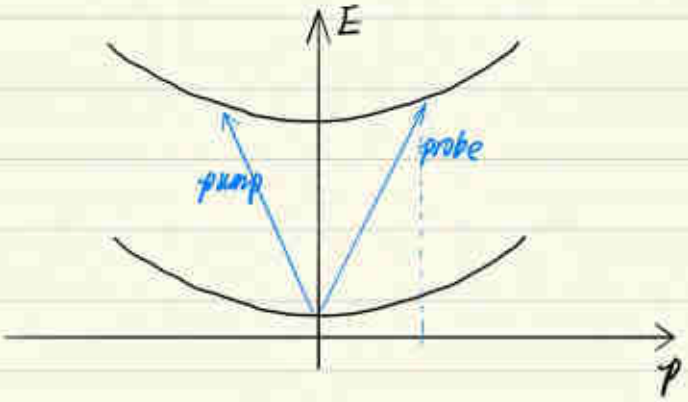
吸收光子后，原子动量会发生改变

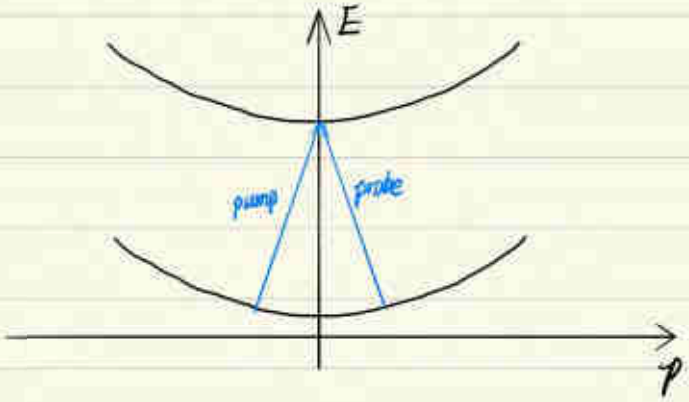
$$E_1 = \frac{p^2}{2m}$$

动能变化 $\Delta E = \frac{(p+\hbar k)^2}{2m} - \frac{p^2}{2m}$

$$= \left(\frac{\hbar k}{2m}\right)^2 + v\hbar k$$







这两种信号强度是同样高的，分布在两侧。合起来以后就没有recoil shift。只有在自然线宽小于这个shift的时候，才能从光谱上面分辨（大部分时候是不行的）

10.2 Phase Sensitive Detection

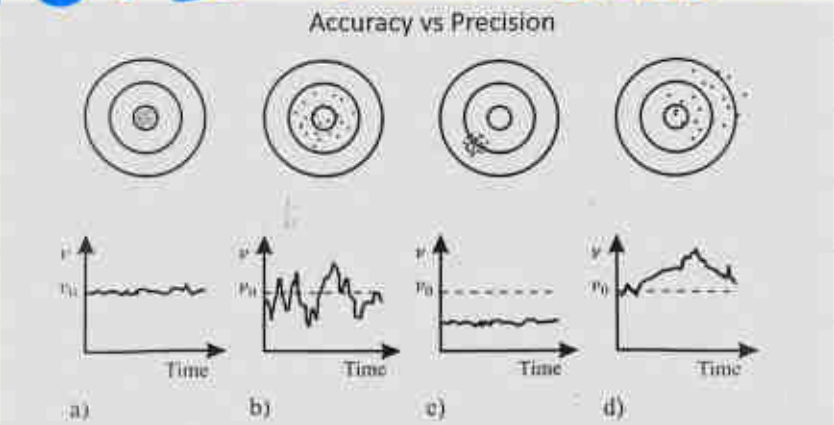
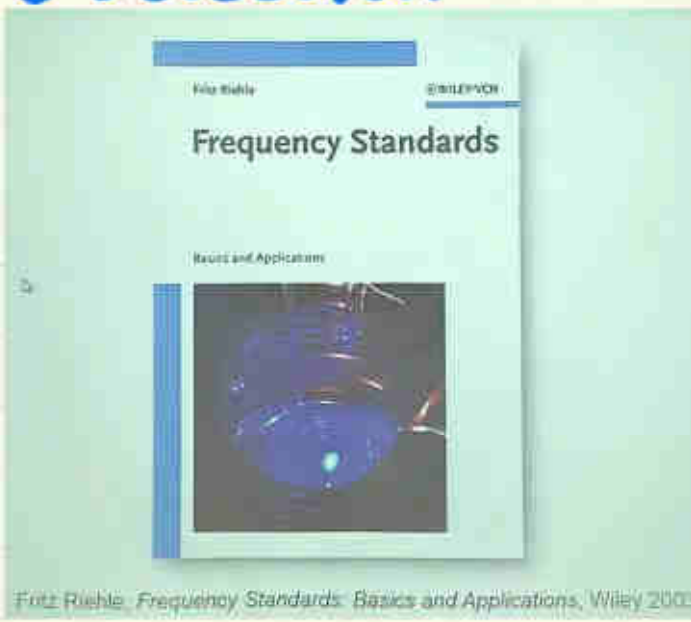


Figure 1.4: Bullet holes on a target (upper row) show four different patterns that are precise and accurate (a), not precise but accurate (b), precise but not accurate (c), not precise and not accurate (d). Correspondingly a frequency source (lower row) shows a frequency output that is stable and accurate (a), not stable but accurate (b), stable but not accurate (c), and not stable and not accurate (d).



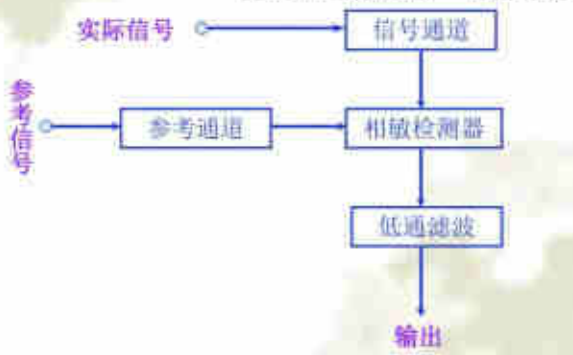
Fritz Riehle, *Frequency Standards: Basics and Applications*, Wiley 2004

PID 对幅度噪声敏感

锁相放大器 (补充量子信息技术)

2、锁相放大器

通过信号通道做一个预处理



Phase Sensitive Detection (PSD)—Lockin amplifier

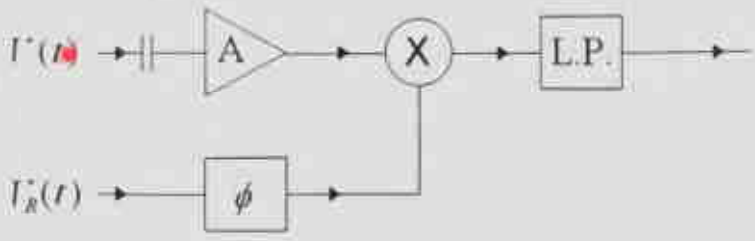
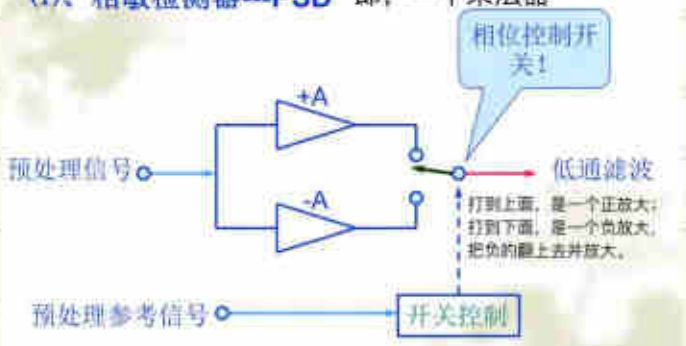
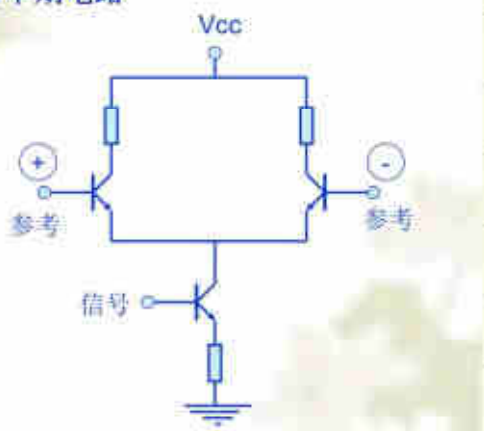


Fig. 1 Block diagram of phase-sensitive detection.

(1)、相敏检测器---PSD 即，一个乘法器

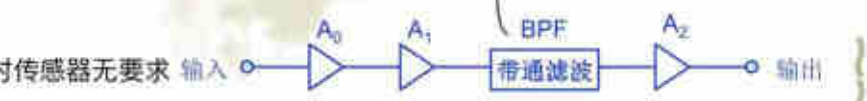


典型的早期电路



(2)、信号通道

不具有放大功能，只具有滤波功能



A_0 —— 前置放大器 pre-amplifier, p-A

负责对来自传感器的信号进行做前期处理！

i）干扰抑制；

ii）阻抗匹配；

iii）增加驱动能力。

不要求有放大倍数。主要目的是阻抗匹配和增加驱动能力。

注意：前置放大器没有通用件，多数情况下要自己做！

电学滤波器隔离度不高，并且衰减厉害，所以这个滤波器之后需要再放一个放大器。

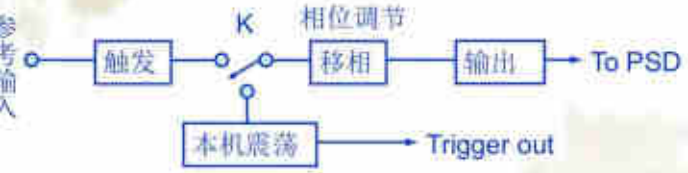
A_1 ---- 多级可变增益放大器

放大倍率可调节，负责对信号再放大，使信号在被BPF衰减后不至于太弱；

A_2 ---- 补偿放大器

放大倍率可调节，负责对信号再放大，使信号能与PSD匹配良好，达到最好的锁相滤波效果！

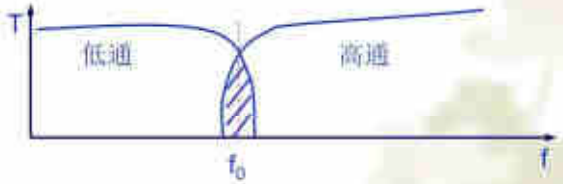
(3)、参考通道



锁相放大器自己带的一个信号

Trigger out 为外部设备提供同步信号用。触发器工作，接到trigger in上。（例如接到激光器上面）

BPF ---- 带通滤波器



低通和高通截止频率可变，f_0 可变--所谓扫频滤波器

notch在电学里面特别需要，特别是在做微弱信号测量的时候。锁相放大器工作时尽量找一个素数的值锁住，例如1331hz这样子。因为空气中有各种各样的噪声。

(4)、低通放大器

比较简单的直流放大器，使实际信号达到外部显示要求！

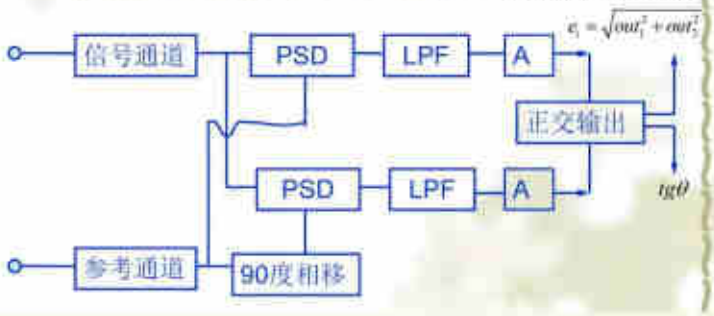
目前新的设备都带有A/D转换，并数字化输出。

3、正交型锁相放大器

（Lock-in Amplifier--LIA）

$\sin^2\theta + \cos^2\theta = 1$

锁相放大器的实际输出：$E=e_s\cos\Delta\theta$ 这样就可以直接给出最大振幅。



一维

散射力：$F = \hbar k R_{scatter} = \hbar k \frac{\Gamma}{2}\left(\frac{I/I_{sat}}{1 + I/I_{sat} + 4\Delta^2/\Gamma^2}\right)$

$F_{max} = \hbar k \frac{\Gamma}{2}$ ，$v_r = \frac{\hbar k}{m}$ ，

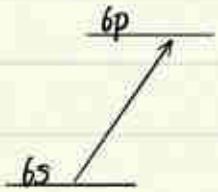
$a_{max} = \frac{\hbar k}{M}\frac{\Gamma}{2} \sim 10^5\ m/s^2$

$L = \frac{v_0^2}{2a_{max}}$

Chapter 11
Laser Cooling and Trapping

11.1 Cycling Transition

激光冷却　　^{133}Cs，6s-6p，850nm



$\frac{h}{\lambda} = m\delta v \Rightarrow \delta v = 3mm/s$

$\left\{\begin{array}{l} ① \text{ absorption} \\ ② \text{ stimulated emission} \end{array}\right\}$ 合效果 $\delta v = 0$

$\left\{\begin{array}{l} ① \text{ absorption} \\ ② \text{ spontaneous emission (spontaneous decay)} \rightarrow \text{average effect } \langle \delta v \rangle = 0 \end{array}\right\}$ 合效果 $\langle \delta v \rangle = 3mm/s$

所以光强增强不是很有用，速率主要取决于自发辐射

最大的光子散射速率：　$\frac{1}{2\tau}$

In the homogenously broadened case, the steady-state solutions again give explicit expressions for the components. The total scattering rate is

$$R_{sc} = \Gamma \rho_{ee}(t \longrightarrow \infty) = \frac{\Gamma}{2}\frac{s}{1+s}, \qquad \text{(total scattering rate)}$$

while the coherent scattering rate is

$$R_{sc}^{(coh)} = \Gamma |\tilde{\rho}_{eg}(t \longrightarrow \infty)|^2 = \frac{\Gamma}{2}\frac{s}{(1+s)^2}. \qquad \text{(coherent scattering rate)}$$

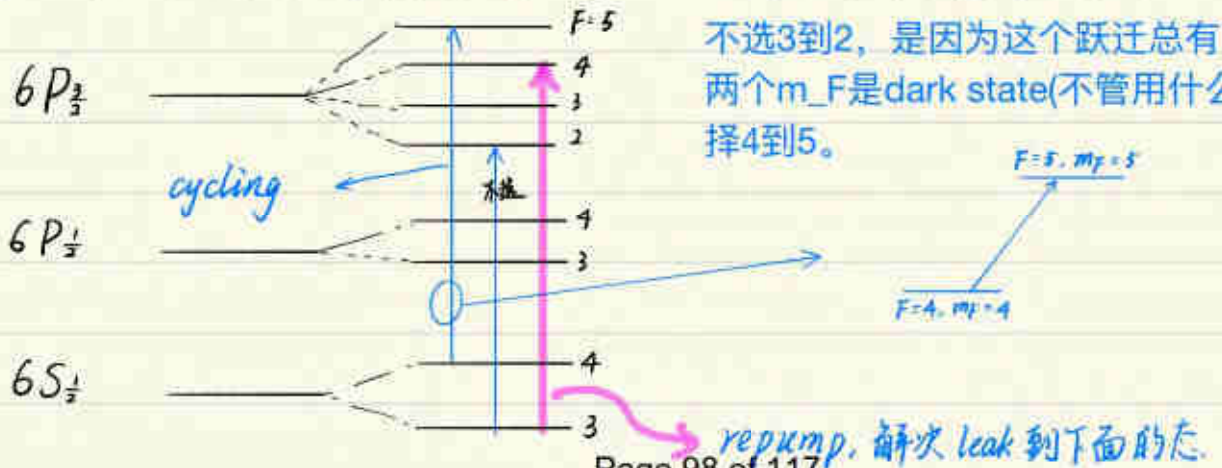
The incoherent scattering rate is the difference of these two expressions:

$$R_{sc}^{(inc)} = R_{sc} - R_{sc}^{(coh)} = \frac{\Gamma}{2}\frac{s^2}{(1+s)^2}. \qquad \text{(incoherent scattering rate)}$$

最大加速度：　$a_{max} = \frac{1}{2\tau}\delta v = 5\times 10^4\ m/s^2$　　$(\tau = 30\,ns)$

stopping distance：　$s = \frac{v^2}{2a_{max}} = \frac{(200\,m/s)^2}{2\times 5\times 10^4\,m/s^2} = 0.4\,m$

所以激发一次是不够的，需要做cycling transition，过程中不能掉到暗态。

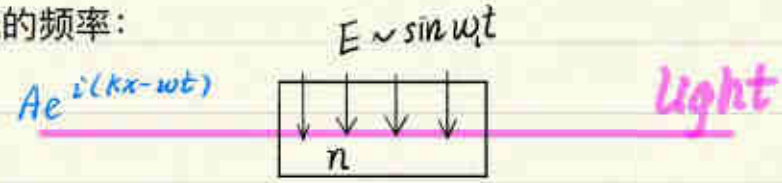


不选3到2，是因为这个跃迁总有两个F=3中的两个m_F是dark state(不管用什么光)。所以选择4到5。

11.2 EOM and AOM

EOM： Electric Optic Modulator

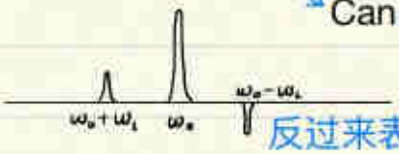
微调激光的频率：



$\Delta\varphi = \frac{2\pi x}{\lambda} = \frac{2\pi n x}{\lambda_0}$ ， n 也是 $\sim \sin\omega_1 t$ 变化

After： $Ae^{-i(\omega_0 t + \varphi_0 \sin\omega_1 t)}$ 相位调制 phase modulation

Can be expanded by Bessel function



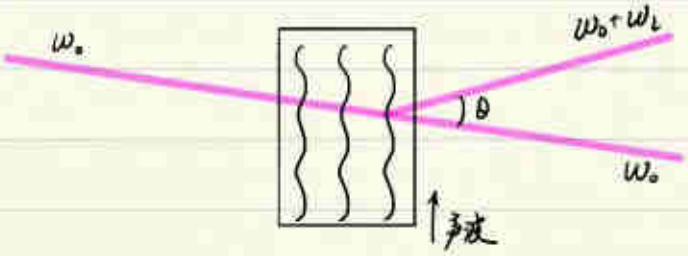
反过来表示，相位相差一个Pi

hyperfine splitting大概是几百MHz，可以通过EOM等调出来。

上面这个相位在repump的时候没用，但是在做PDH稳频的时候有用。

AOM： Accousto Optic Modulator

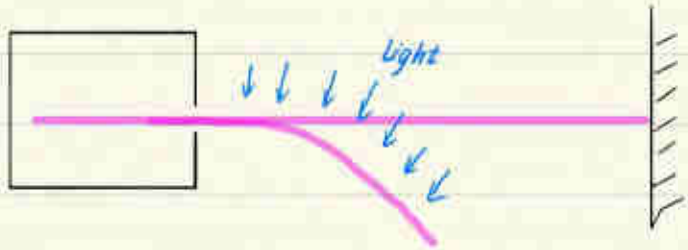
也是通过一种晶体，PCT晶体 一般指锆钛酸铅压电陶瓷



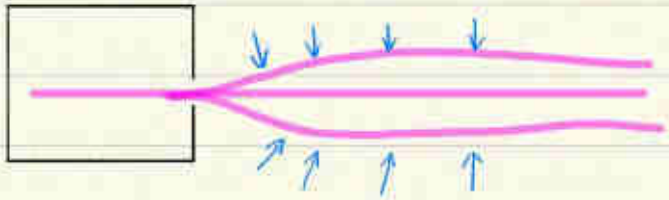
声波的传播造成密度的差异，形成一个光栅，这样就出现了衍射。由于这个光栅是在向上移动的，被运动的声波衍射的光的频率会发生变化，变化的频率就是调制的频率。

11.3 Zeeman slower

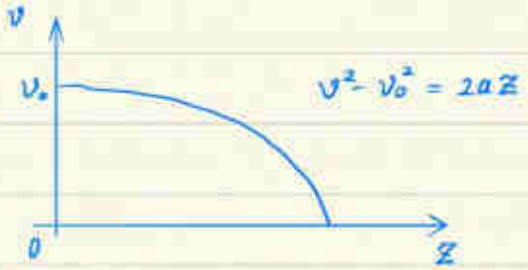
让原子转弯　　原子转弯之后，光也必须转，以保证共振。否则转过去之后多普勒位移与自然宽相当的时候，就不共振没办法继续转弯了。



transverse cooling：增加向前的原子数目，让两边的原子都转一下，相当于聚焦准直。



longitudinal cooling　　slowing



但是原子减速的过程中，由于多普勒效应，原子并不会始终共振。那么就有两种想法，一种调节激光，另一种调节能级差。

Chirping：调节激光频率的方法

Zeeman Slower

用Zeeman效应抵消多普勒频移　　保持 $\Delta\omega_{Zeeman} = \Delta\omega_{Doppler}$

用一个不均匀的磁场，一个长筒，绕线不是均匀的。

优势：原子不是一股一股的，而是连续的。

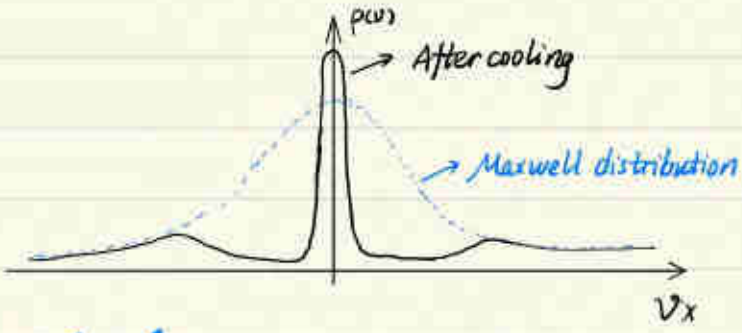
如果初速度减速，线圈仍然可以用。

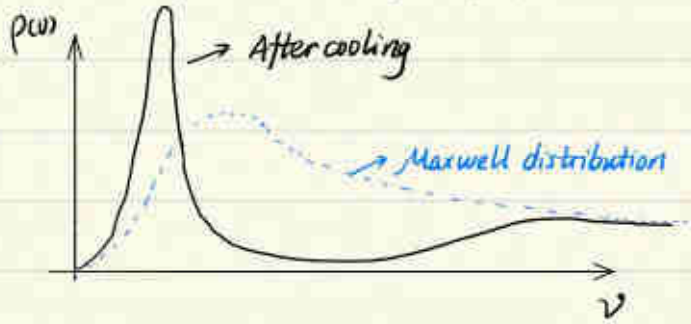
该速度以下的可以捕获

$$\rho(v)\,dv \propto e^{-(\frac{v_x}{u})^2} e^{-(\frac{v_y}{u})^2} e^{-(\frac{v_z}{u})^2} dv_x\, dv_y\, dv_z \propto v^2 e^{-(\frac{v}{u})^2} dv$$

$\langle \frac{1}{2} m v_x^2 \rangle = \frac{1}{2} k_B T$ 也可以看作是温度的定义

(更严谨: $\frac{1}{2} m \langle (v_x - \langle v_x \rangle)^2 \rangle = \frac{1}{2} k_B T$. 取决于 v_x 的 spread 而不是自身 v_x 数值)



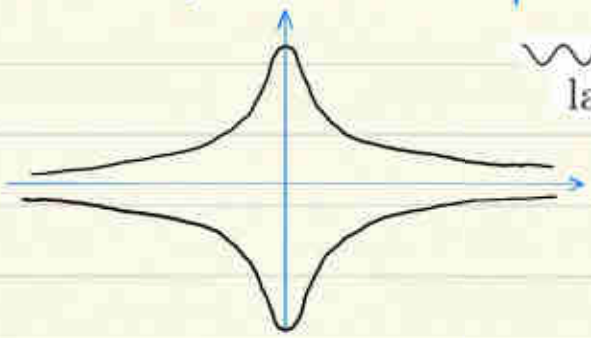


11.4 Doppler Cooling

$$F = -\alpha v = m\frac{dv}{dt} \Rightarrow -\alpha v^2 = \frac{1}{2} m \frac{d(v^2)}{dt} \Rightarrow -\frac{2\alpha}{m} E = \frac{dE}{dt} \Rightarrow E = E_0 e^{-(\frac{2\alpha}{m})t}$$

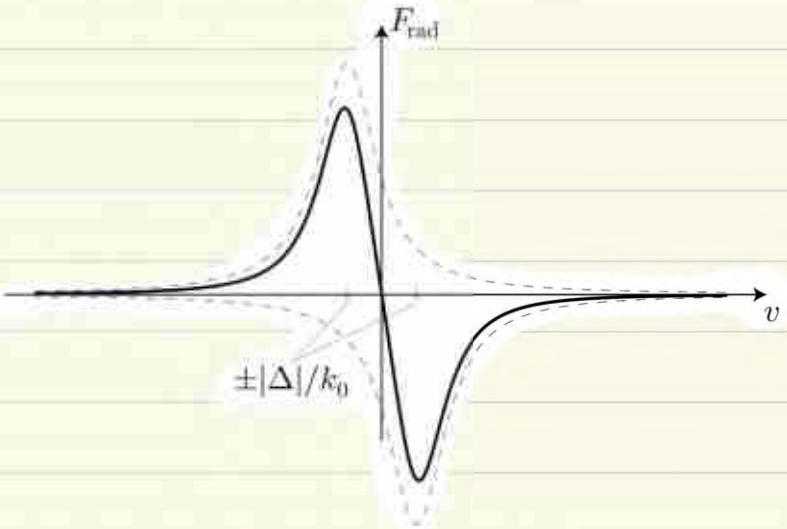
上面散射力: $F = \frac{h}{\lambda}\frac{n_e}{\tau} = \frac{h}{\lambda}\frac{1}{2\tau}\frac{I/I_s}{1 + I/I_s + 4\frac{\Delta^2}{\Gamma^2}}$, $\Delta = \omega_L - \omega_0 \pm kv$

如果 $\Delta = \omega_0 - \omega_L = 0$. 那么打相对的两束光, 都是 Lorentz lineshape:



这种不失谐的情况，力就相互抵消了

为了获得 $\vec{F} \propto -\vec{v}$ 的力, 调至红失谐(频率减小)



(如果是blue detuning的话，就变成正的斜率了，就会加热原子)

Doppler Cooling的下限

存在涨落，这种随机性造成heating

$$v_{i+1} = v_i \pm \delta v, \qquad \langle v_{i+1} \rangle = \langle v_i \rangle$$

$$\langle v_{i+1} \rangle^2 = \langle v_i \rangle^2 + \langle \delta v \rangle^2 \qquad \text{造成加热（动能增加）}$$

$$\Delta E = \frac{1}{2} m (\delta v)^2$$

散射率+吸取率

$$\begin{cases} \text{加热} & \dfrac{dE}{dt} = \left[\frac{1}{2} m (\delta v)^2\right] R \\ \text{冷却} & \dfrac{dE}{dt} = -\left(\frac{2\alpha}{m}\right) E \end{cases}$$

⇒ Doppler Cooling Limit:

where k_B is the Boltzmann constant. This gives

$$k_B T = \frac{\hbar\gamma}{4} \frac{1 + (2\Delta/\gamma)^2}{(-2\Delta/\gamma)}. \tag{1.111}$$

当 $\Delta = -\frac{\Gamma}{2}$ 时最低

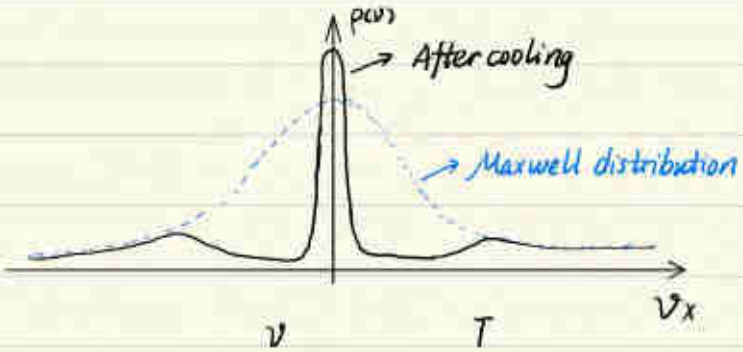
The temperature is minimized for the detuning $\Delta = -\gamma/2$, giving the **Doppler temperature** T_D:

$$k_B T_D = \frac{\hbar\gamma}{2}. \tag{1.112}$$

(Doppler limit)

对 ^{133}Cs, $T_D = \frac{\hbar\gamma}{2k_B} = 150\ \mu K$

几个速度



	v	T	
Thermo	200 m/s	300 K	$u = \sqrt{\frac{2k_B T}{m_{Cs}}}$
Capture	5 m/s		$k v_{capture} = \Gamma = 2\pi \cdot 6\ \text{MHz}$
Doppler Limit	0.15 m/s	150 μK	$k_B T_{Doppler} = \frac{1}{2}\hbar\Gamma$

对于原子钟等来讲，这个速度还是太大了。

11.5 Sub-Doppler Cooling

Sisyphus Cooling (=polarization gradient cooling)

仍然会受到反冲的影响（recoil）

$$v_r = \frac{h}{\lambda}\frac{1}{m_{Cs}} = 0.003\ m/s \xrightarrow{\text{对应}} 100nK$$

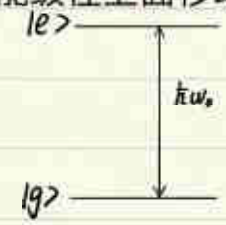
现在实验上做到 $1\mu K$

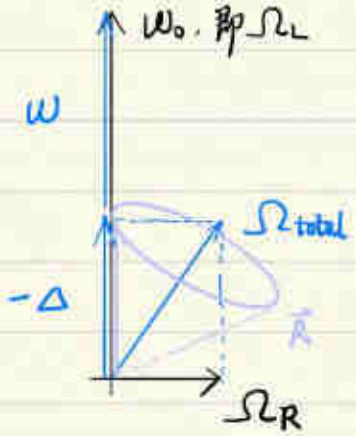
如果如果想要更低，就不能靠光来激发原子：Evaporative Cooling

需要设想一种办法，密度比较高，并且不靠激光把原子囚禁，能达到pK

利用Light Shift（AC Stark Shift）

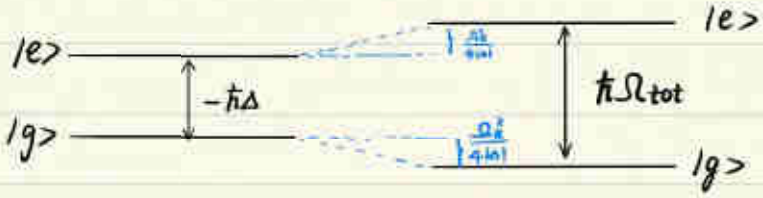
打红失谐的光，下面能级往下面移动，上面能级往上面移动





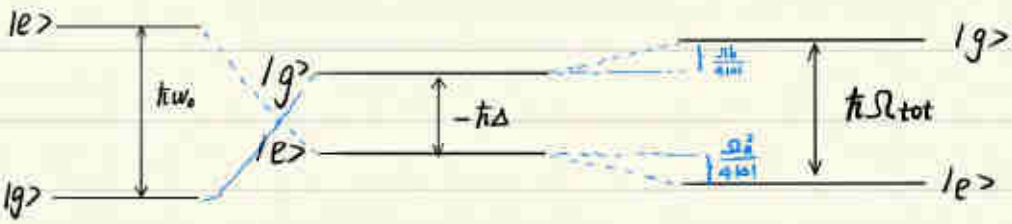
跳到光频率即omega的场上，在旋转场中：

考虑到光的影响：

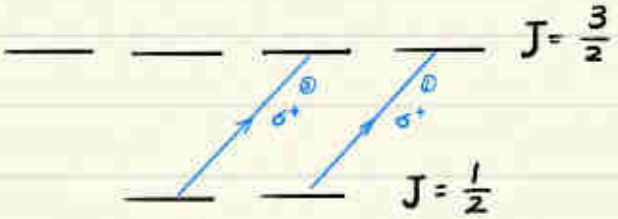


$$\delta\omega = \sqrt{\Delta^2+\Omega_R^2} - |\Delta| \xrightarrow{\Delta \gg \Omega_R} \frac{\Omega_R^2}{2|\Delta|}$$

蓝失谐的光，下面能级往上面移动，上面能级往下面移动



吸引原子的话，需要red detuning，如果想要排斥原子，需要blue detuning

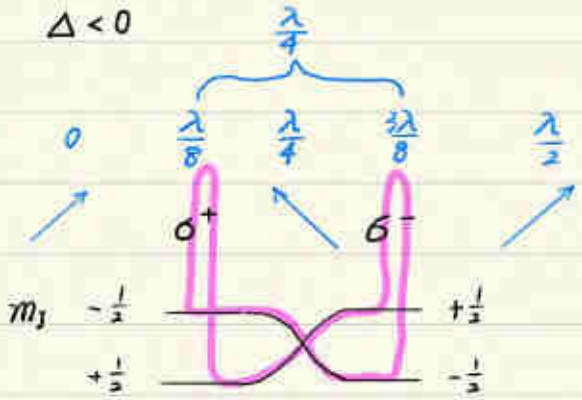


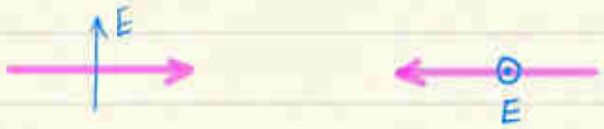
① $\langle \frac{1}{2}\frac{1}{2}11 | \frac{3}{2}\frac{3}{2} \rangle = 1$,

② $\langle \frac{1}{2}-\frac{1}{2}11 | \frac{3}{2}\frac{1}{2} \rangle = \frac{1}{3}$

而light shift正比于Rabi Freq的平方，故正比于CG系数的平方

$\Delta < 0$





相位随空间变化的空间周期是 lambda/2

光的强度要弱一点

到这样温度下，做fountain clock够了，但是做BEC还不够

11.6

突破recoil limit

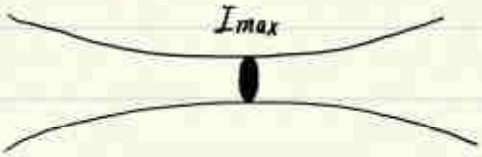
Optical Dipole Trap

陷深 $Depth = \frac{\Omega_R^2}{4|\Delta|} \propto \frac{I}{|\Delta|}$

激发率 $R \propto \frac{I}{\Delta^2}$ $\left(R = \frac{\Gamma_{sp}}{2} = \frac{1}{2\tau} \frac{1}{1+\frac{I}{I_s}(1+4\frac{\Delta^2}{\Gamma^2})} \xrightarrow{\Delta^2 \gg \Gamma^2} \frac{I}{\Delta^2} \right)$

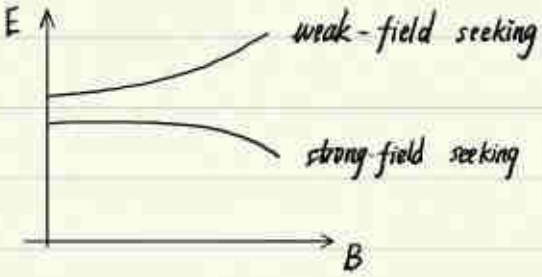
Use high intensity and far detuning light.

原子会囚禁在光强度最大的地方



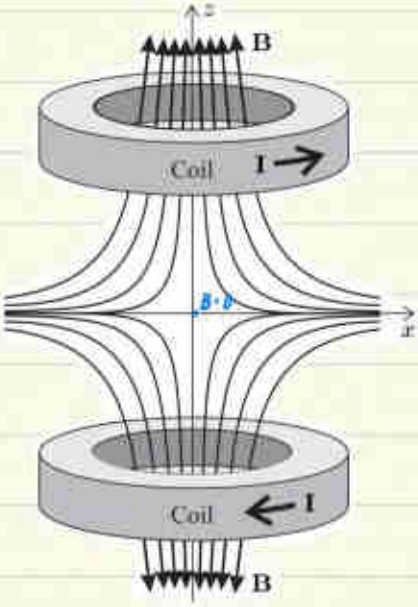
11.7

Magnetic Field Trap



$B_{center} = \langle B_{sphere} \rangle$，故不可能有真空中 B_{max}。

但是极小值是可以的，例如用一个anti-Helmholtz coil。

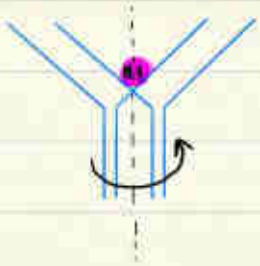


利用这种，可以抓处在weak-field seeking态的原子

但是当两个态简并的时候，就有可能flip，即在B=0的地方。如果翻了之后，就会变成strong field seekin跑掉。就相当于是一个漏斗。

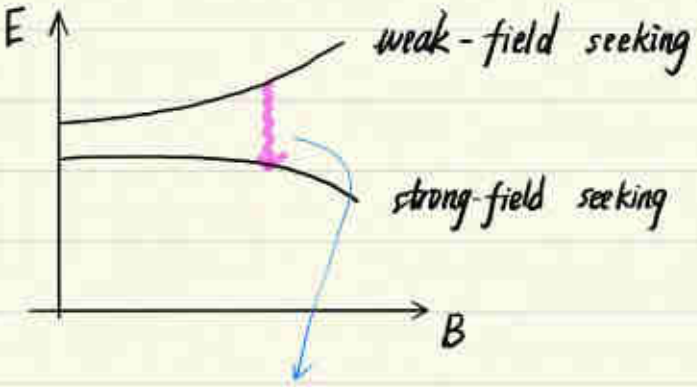
方法一：在中间那个位置打一束光，不能激发原子并且把原子推开，需要一个blue detuning的光

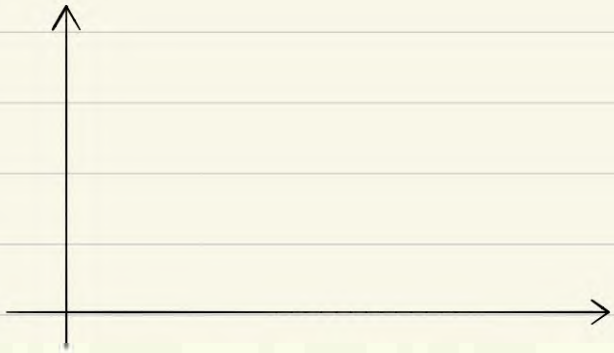
方法二：把这个漏斗转起来，只要转的足够快，原子就跟不上，只能在一个中间位置：



11.8

Evaporative Cooling



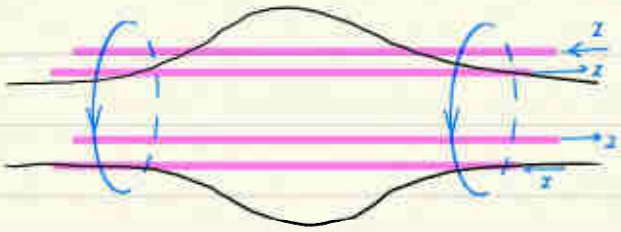


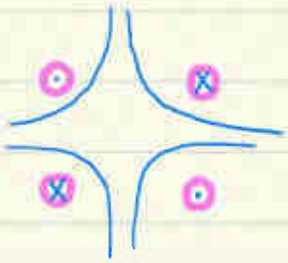
多加一个射频磁场，诱导在某一个位置的从weak field seeking到strong field seeking的跃迁。这样位置外围（对应磁场强的地方）一过来，就会掉到下面，然后跃迁掉。重新达到热平衡的过程，分布会重新分布，整体温度会降低。然后温度高的再次跑掉，重复这个过程。要求达到热平衡要足够快。

11.9

Magnetic trap

侧向磁场由四根杆提供，轴向磁场由Helmholtz线圈提供（这里是同向的），于是就不会有B=0的点。不会造成spin flip。



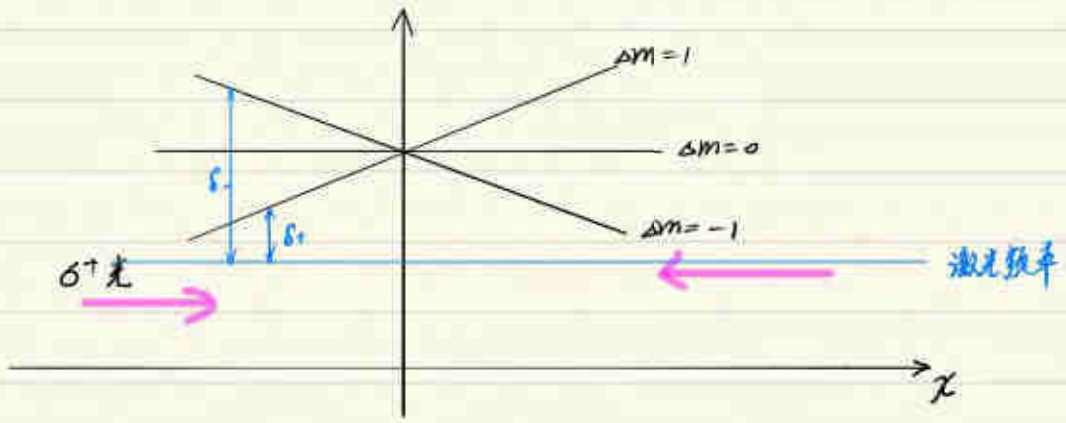


11.10

Magnetic-optical Trap (MOT)

需要一个Zeeman效应

一维情况，使用一个红失谐的光，并且指定偏振。偏振和磁场方向配合好就能囚禁。



这样，对于左边的原子来说（x<0的地方），对sigma+的光失谐量小，光子吸收（散射）率高，而对向左传播的sigma-的光失谐量大，光子吸收（散射）率低，所以净效应是吸收向右传播的光更多，受到一个指向原点的回复力。右边也是同理。

$F = -\alpha v - kx$ → 回复力，力开始与位置有关，由而能囚禁

11.11

Dipole Trap　　只有囚禁的功能，没有冷却的功能

AC- stark

用光形成一个势阱

$$U = \frac{\Omega^2}{4\delta} = \frac{\hbar\Gamma}{\gamma}\frac{I}{I_{sat}}\frac{\Gamma}{\delta} \propto \frac{\Gamma}{\delta}$$

$$R_{scatter} = \frac{\Gamma}{\delta}\frac{I}{I_{sat}}\left(\frac{\Gamma}{\delta}\right)^2 \propto \frac{\Gamma}{\delta^2}$$

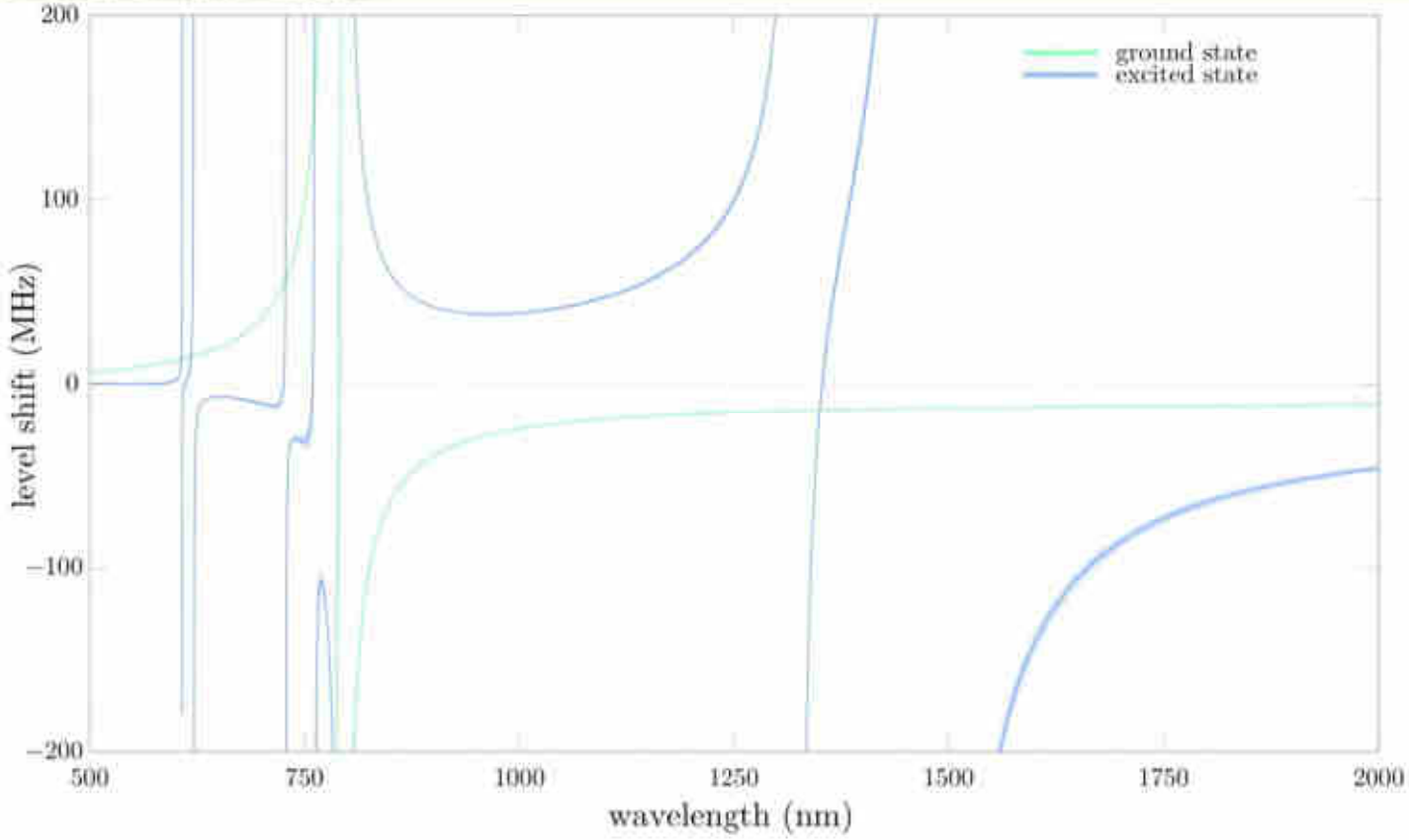
所以必须减少加热的机制，让光子散射率降下来。所以要调大失谐，调的很大。所以光强都需要非常强。

这样子能玩的花样比较多，比如形成周期性的double well，或者lattice等。

11.12 Magic Wavelength

In the two-level atom, the ac Stark shift always results in opposite shifts between the excited and ground states, and thus always leads to a shift of the transition frequency. Of course, the fact that couplings to other states exist can work to our advantage. In particular, when accounting for the counterrotating interactions and couplings to other levels, it may be possible to find situations where the excited- and ground-state shifts are equal, with the *same* sign. This situation happens when the atom is driven at particular wavelengths, called **magic wavelengths**.

To illustrate this, consider the level shifts of ^{87}Rb of the two levels in the D_1 transition at 794 nm due to a monochromatic laser field.



The plotted energy shifts correspond to those experienced by an atom at the center of a 1 W Gaussian beam of radius $w_0 = 10\ \mu$m. We will defer the details of the calculation until we develop more sophisticated technology for dealing with atomic structure. For now, we will note that we have done the calculation accounting for 24 total atomic transitions, some of which are visible as dispersive resonances in the level-shift curves. Magic wavelengths occur at the locations where the two curves intersect. For example, a laser spot at 1350.39(65) nm can be used as a dipole trap for ^{87}Rb, where the frequency of the D_1 transition is not affected.

Why is this interesting? There are two well-known application. The first is, suppose you have an atom in a dipole trap, and you want to probe a transition with a resonant laser. Well, recall that the stochastic dipole force is due precisely to having different dipole potentials in different states, and then stochastically jumping between them due to spontaneous emission. Of course, the same thing will happen in this situation: when probed, the atom will jump between the ground and excited states, where it will experience different trapping potentials. This can be a large source of heating and decoherence. But trapping at the magic wavelength suppresses this form of heating. This approach is used to great advantage in cavity quantum electrodynamics to obtain long trap lifetimes of a single atom in an ultrahigh-finesse cavity.[47]

The other application is to atomic frequency standards. The current frequency standard is based on a microwave hyperfine transition in ^{133}Cs. But increasing the quality factor $\omega_0/\delta\omega$ of the oscillator standard requires both decreasing the line width $\delta\omega$ as well as pushing the resonance frequency ω_0 into the optical. To allow for long interrogation times, the atoms must be trapped. One promising approach is the single-ion atomic clock, where the oscillating trap fields average to zero to lowest order. Another promising approach is to trap atoms in a magic-wavelength, three-dimensional optical lattice.[48] This allows the atoms to be trapped with little shift of the optical transition. Also, the atoms do not suffer collisions because they are isolated at different lattice sites. So the clock does not suffer from a collisional shift, but retains the advantage of averaging over many atoms.

11.13

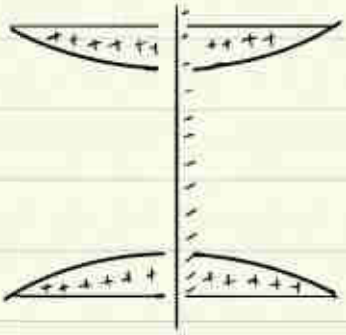
离子的囚禁

原子	离子
Light force	electric field force
$\frac{\hbar k}{m}\frac{1}{2\tau} \sim 10^5 m/s^2$	$\frac{eE}{m} \sim 10^{10} m/s^2$

$\nabla^2 E = 0$ It is impossible to use only static electric field to trap ions.

Knight trap

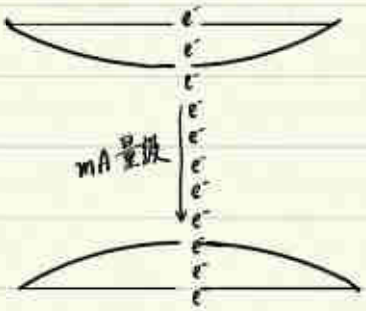
中间有一个丝，所以如果角动量比较大就碰不到那个丝；但是一旦离子温度冷下来之后，就会碰到丝就不行了。



Electron Beam Ion Trap

没有那根丝了，取代为电流很大的电子束流

可以用来捕获高电离态的离子（比如只剩下一个裸核），也可以用来产生高电离态的离子（直接轰没）

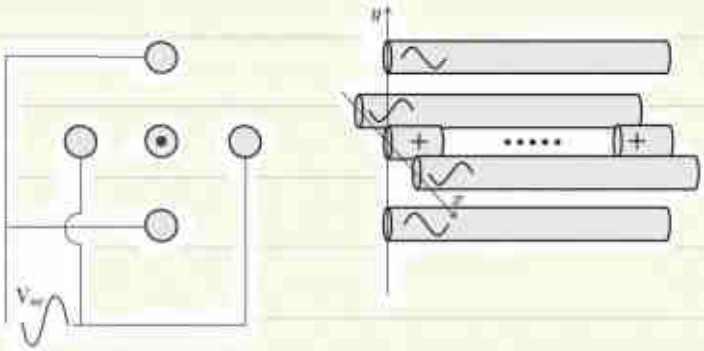


Paul Trap

$$m\ddot{x} = QE_0 \sin(\omega t)$$

$$\Rightarrow \quad x_0 = -\frac{QE_0}{m\omega^2}$$

But E_0 is not a constant. It is a function of place.



在一个点上求电场的平均值，肯定是0.但是这里需要跟着离子跑，关心离子感受到的电场的平均值。这里Paul Trap有了电场梯度，所以就有可能了。

把离子的运动展开，考虑一个慢变的项，加上一个正弦项

$$E_0 \rightarrow E_0(x)$$

$$\begin{cases} x = x_s + x_f \sin\omega t \quad \Rightarrow \quad \ddot{x} = \ddot{x}_s - x_f\omega^2 \sin\omega t \\ E(x) = E(x_s) + \left.\frac{dE}{dx}\right|_{x_s} x_f \sin\omega t \end{cases}$$

代入 $m\ddot{x} = QE(x)\sin\omega t$

$$\Rightarrow \quad m\ddot{x}_s - m x_f \omega^2 \sin\omega t = QE(x_s)\sin\omega t + Q\frac{dE}{dx} x_f \sin^2\omega t$$

$$x_f = -\frac{Q}{m\omega^2}E(x_s)$$ micromotion 微运动，一个快速的抖动，时间平均为0.

剩下方程 $m\ddot{x}_s = Q\frac{dE}{dx}x_f \sin^2\omega t \xrightarrow{\langle\sin^2\omega t\rangle = \frac{1}{2}} Q\frac{dE}{dx}x_f\frac{1}{2}$

$$\Rightarrow \quad \ddot{x}_s = -\frac{Q^2}{4m^2\omega^2}\frac{d(E^2)}{dx}$$ Drift 时间平均不是0，力就出来了。

力指向电场小的方向，与电场的方向无关，与离子的正负也无关。

频率的计算

四极杆的电场：

$\vec{E} = -\frac{V_0}{r_0^2}(\vec{x}-\vec{y})\sin(\omega t)$, $\frac{dE^2}{dx} \propto x$ Harmonic potential

$$\omega_{trap} = \sqrt{\frac{k}{m}} = \frac{|Q|V_0}{\sqrt{2}m\omega r_0^2}$$

如果想要保证离子的束缚势稳定的，必须保证离子的运动和电场的方向相反，即上面的频率小于外场的频率：

Stability : $\omega_{trap} = \frac{|Q|V_0}{\sqrt{2}m\omega r_0^2} < \omega$

事实上，上面都是近似，并且是一个一维的模型。

书上有精确解：

Quadrupole Mass Spectrometer（QMS）

所以离子想要被囚禁，必须有足够重的质量。存在一个质量的下限。

Trap stability -> Lower mass limit

而从井深的角度来讲，太重了也不好：

$U \sim \frac{1}{2}k_{trap}r^2$. $k_{trap} \propto \frac{1}{m}$

通过加直流电压，存在一个upper mass limit

所以对质量的选择性，可以用来做质谱仪（卖钱）

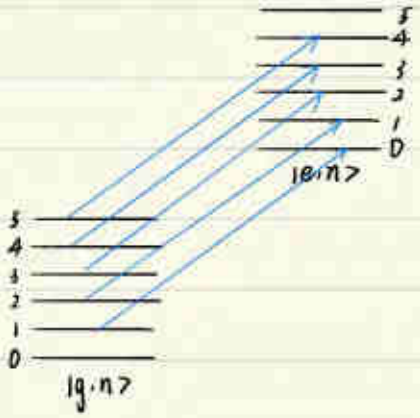
当打开U即直流电压的时候，a就不为零，这时候那条直线就出现，就出现了质量范围。

Residue gas analyzer（RGA）

做原子钟的用Sr，外面有两个电子：原因是有两个对环境条件很不敏感的态。
做离子钟的用Al，打掉一个电子剩下两个电子。

Buffer Gas Cooling

Sideband Cooling $\Omega_{trap} \sim MHz$



excitation: $|g,n\rangle \longrightarrow |e,n-1\rangle$. 频率 $\omega_0 - \Omega_{trap}$

Sideband Cooling的一个要求是: $\Omega_{trap} > \Gamma$

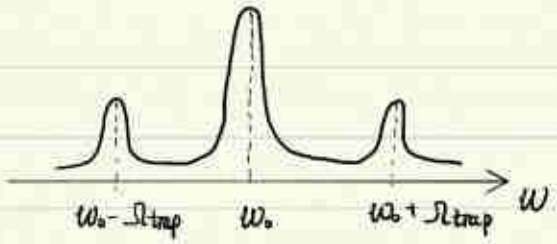
这样就几乎不会跃迁到别的地方

所以一般都把阱做的很深，这样Omega_trap也大

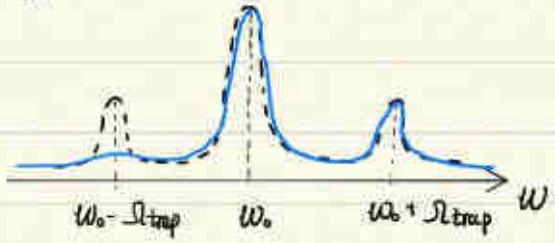
$\langle e,\phi_m | \hat{H} | g,\phi_n \rangle = \langle e|\hat{H}|g\rangle \langle \phi_m|\phi_n\rangle \propto \delta_{mn}$ 近似的选择定则: $\Delta n = 0$

跃迁的，$\hat{H} \propto e\vec{r}\vec{E}e^{-i\omega t}$，与原子空间位置近似无关，故可把 $\langle\phi_m|\phi_n\rangle$ 拿出.

激发的时候由于有一个光子的反冲 $\phi_m(p) \rightarrow \phi_n(p \pm \frac{k}{\lambda})$ 不太符合近似的选择定则



冷却到振动基态



red sideband
$|n\rangle \rightarrow |n-1\rangle$

blue sideband
$|n\rangle \rightarrow |n+1\rangle$

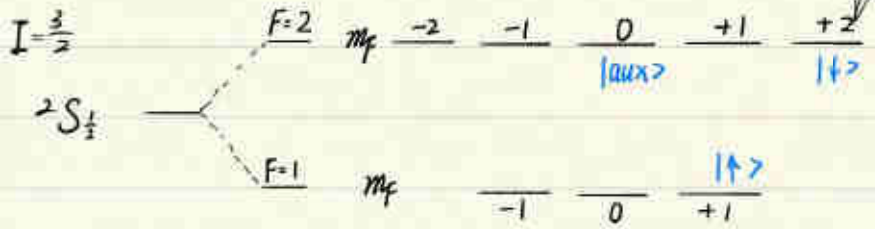
Controlled-Not Gate

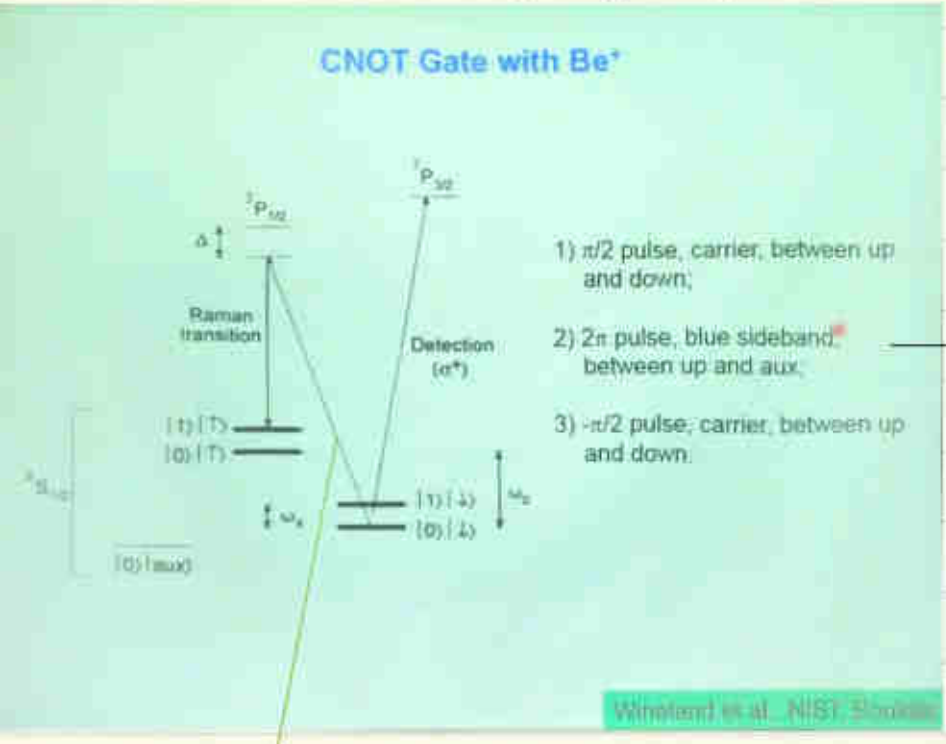
	control	signal
	$\|0\rangle$	$\|0\rangle$
$\xrightarrow{\text{control } \frac{\pi}{2} \text{ pulse}}$	$(\|0\rangle + \|1\rangle)\|0\rangle$	Quantum superposition
$\xrightarrow{\text{CNOT}}$	$\|0\rangle\|0\rangle + \|1\rangle\|1\rangle$	Quantum entanglement

$^2P_{\frac{3}{2}}$, $F=3$, $m_F=3$

cycling transition ; detection

如果在down，就是亮的，如果在up，就是暗的





只作用于 $|0\rangle|aux\rangle \leftrightarrow |1\rangle|\uparrow\rangle$，

这样只有 $|1\rangle|\uparrow\rangle$ 增加了负号，

然后经 $-\frac{\pi}{2}$ 变成 $|1\rangle|\downarrow\rangle$

$|0\rangle|\uparrow\rangle$ 不增加负号，

然后经 $-\frac{\pi}{2}$ 回到原位 $|0\rangle|\uparrow$

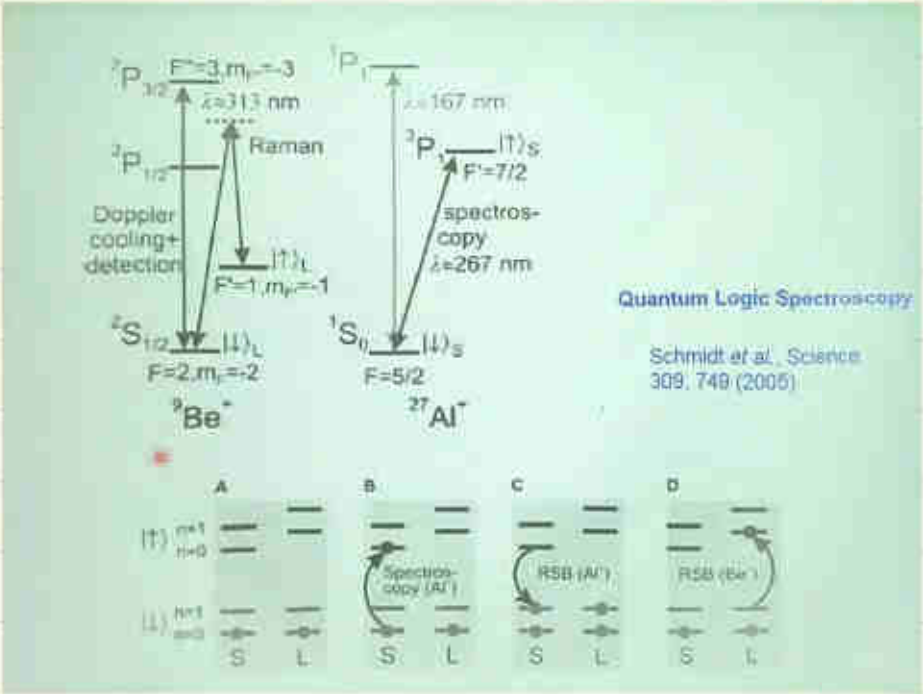
实现了 CNOT 门

大的红失谐，防止激发E1跃迁，避免spontaneous emission

11.14

Sympathetic Cooling

通过原子的弹性碰撞（或者离子之间的斥力），让容易冷却的粒子冷却不容易冷却的粒子



Al^+，利用 $^1S_0 \to {}^3P_0$ 跃迁做钟

clock transition

这是一个E1禁戒的跃迁，线宽非常窄。

Be离子不仅可以冷却，还可以用来读出Al离子的内态处于哪一个态。

Quantum Projection Noise

$$\sigma^2 = N n_e (1-n_e)$$

$n_e \approx \frac{1}{2}$ 时，$\sigma \propto \frac{\sqrt{N}}{2}$

$\Rightarrow$ Signal $\sim N$，noise $\sim \sqrt{N}$，$SNR \propto \sqrt{N}$

$N=1$，$|g\rangle + |e\rangle e^{-i\omega t}$

$N=3$，$(|g_1\rangle + |e_1\rangle)(|g_2\rangle + |e_2\rangle)(|g_3\rangle + |e_3\rangle)$

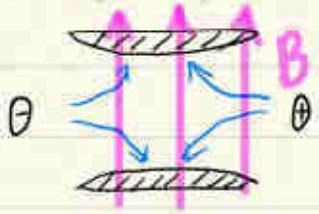
$|g_1 g_2 g_3\rangle + |e_1 e_2 e_3\rangle e^{-3i\omega t}$

算 Signal 时按 $N=3$，算 Noise 与 N 无关 $(N=1)$，$SNR \propto N$

7.13

电子阱 Penning Trap

电场是quadruple



$$m r \omega^2 = Q r \omega B$$

$$\Rightarrow \quad \omega_c = \frac{QB}{m} \qquad \text{cyclotron}$$

$$\begin{cases} F_z = -kz \\ F_r = +\frac{1}{2}kr \end{cases} \Rightarrow \quad \omega_z = \sqrt{\frac{k}{m}}$$

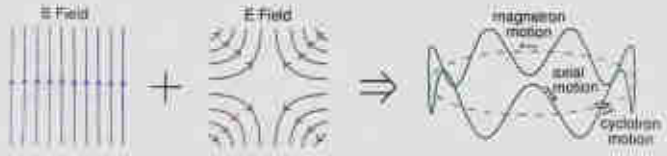
$$m r \omega^2 = QBr\omega - \frac{1}{2} m \omega_z^2 r$$

$$\Rightarrow \quad \omega_\pm = \frac{1}{2}\left[\omega_c \pm \sqrt{\omega_c^2 - 2\omega_z^2}\right]$$

$$\omega_c \gg \omega_z \quad \begin{cases} \omega_+ \approx \omega_c & \text{cyclotron} \quad \text{GHz} \\ \omega_- \approx \frac{\omega_z^2}{\omega_c} & \text{magnetron} \quad \text{MHz} \end{cases}$$

存在两种频率对应的稳定运动

A single electron in a Penning trap

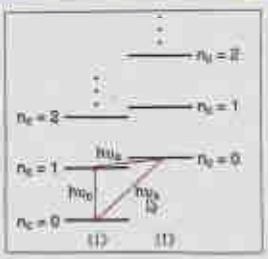


motion	frequency	$h\nu/k_B$	damping
axial	200 MHz	9.6 mK	1 Hz
cyclotron	149.0 GHz	7.2 K	0.02 Hz
spin	149.2 GHz	7.2 K	10^{-12} Hz
magnetron	130 kHz	6.4 μK	10^{-17} Hz

g-factor measurement

g in free space:

$$g = \frac{\overset{\mu}{\mu_B}}{\underset{\hbar}{S}} = \frac{2\mu}{\mu_B} = \frac{\hbar\omega_s}{B\mu_B} = \frac{2\omega_s}{\omega_c}$$



g-2 in free space:

$$\frac{g}{2} = 1 + \frac{g-2}{2} = 1 + \frac{\omega_a}{\omega_c}$$

(3 orders of magnitude for free)

g-2 in a Penning trap:

$$\frac{g}{2} = 1 + \frac{\bar{\omega}_a - \bar{\omega}_z^2/2(\bar{\omega}_c + \frac{1}{2}\delta)}{(\bar{\omega}_c + \frac{1}{2}\delta) + \bar{\omega}_z^2/2(\bar{\omega}_c + \frac{1}{2}\delta)}$$

[Brown and Gabrielse, Rev. Mod. Phys. 58, 1 (1986)]

11.16

Dissipation and quantum noise: the Heisenberg-Langevin approach

The quantum description of random processes is closely related to the theory of random fluctuations in classical statistical mechanics. To motivate subsequent development of the quantum mechanical theory, we will briefly review the classic problem of Brownian motion.

8.4.1 Brownian motion

Consider a heavy particle surrounded by a bath of lighter particles. As the heavier particle moves through the cloud, its interactions with the lighter particles produce a viscous drag, slowing it down. However, the heavy particle never quite comes to rest because it is constantly bombarded by random momentum kicks inflicted by the lighter particles. At long times, the heavy particle will approach thermal equilibrium with its bath.

The Langevin equation

This classic problem of Brownian motion is described mathematically by the Langevin equation, which models the force on the heavy particle as a viscous drag plus a fluctuating "Langevin force",

$$\frac{d}{dt}p = -\eta p + f(t), \tag{8.34}$$

where η is the friction coefficient and $f(t)$ is the random force due to collisions between the heavy and light particles. On average, the Langevin force vanishes,

$$\langle f(t) \rangle = 0 \tag{8.35}$$

and we define its two-time expectation value

$$\langle f(t) f(t') \rangle = 2Dg(t-t') \tag{8.36}$$

in terms of a diffusion coefficient D and a second order correlation function $g(t-t')$ which satisfies the normalization condition

$$\int_{-\infty}^{\infty} g(t-t')dt = 1. \tag{8.37}$$

Note that the time dependence of $g(t-t')$ is determined by the collision frequency. We will be particularly interested in the situation where the lighter particles collide frequently with the heavy particle, but the effect of each collision is small. The heavy particle will thus lose momentum slowly, but the random force $f(t)$ will fluctuate very quickly. In this rapid-collision limit, we can separate out the two timescales, and the correlation function approaches a delta function

$$g(t-t') \to \delta(t-t'). \tag{8.38}$$

We can find a general solution to Langevin equation for arbitrary $f(t)$,

$$p(t) = p(0)e^{-\eta t} + \int_0^t dt' f(t') e^{-\eta(t-t')}. \tag{8.39}$$

If we average the momentum of the heavy particle over timescales large compared to the collision rate, we get

$$\overline{p(t)} = \overline{p(0)e^{-\eta t}}, \tag{8.40}$$

so the average momentum is unaffected by the Langevin force. However, its variance will have contributions from the stochastic momentum kicks. In the rapid collision limit, we can calculate the mean square momentum:

$$\begin{aligned}
\overline{p^2(t)} &= \langle\left(p(0)e^{-\eta t} + \int_0^t dt' f(t')e^{-\eta(t-t')}\right)^2\rangle && (8.41)\\
&= \overline{p(0)^2}e^{-2\eta t} + \int_0^t\int_0^t dt'dt''\langle f(t')f(t'')\rangle e^{-\eta(t-t')}e^{-\eta(t-t'')} && (8.42)\\
&= \overline{p(0)^2}e^{-2\eta t} + \int_0^t\int_0^t dt'dt''2D\delta(t'-t'')e^{-\eta(t-t')}e^{-\eta(t-t'')} && (8.43)\\
&= \overline{p(0)^2}e^{-2\eta t} + \frac{D}{\eta}\left(1-e^{-2\eta t}\right). && (8.44)
\end{aligned}$$

Note that the terms linear in $\rangle f(t)\langle$ vanish because the average Langevin force is zero. This calculation shows that, unlike the average velocity, the mean square momentum is affected by the presence of the diffusion term. For very short times $\eta t \ll 1$, the square momentum simply decays exponentially,

$$\overline{p(t)^2} \approx \overline{p(0)^2}e^{-2\eta t}. \tag{8.45}$$

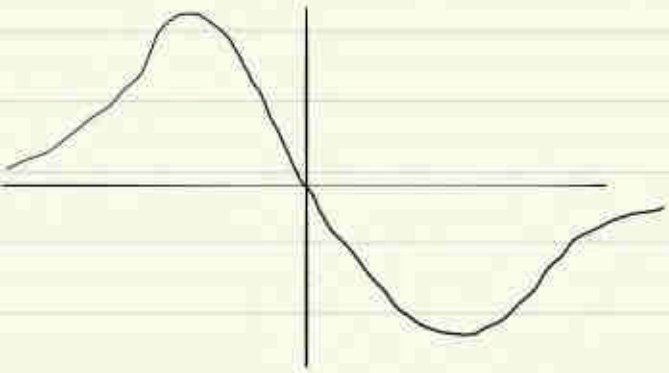
For long times $\eta t \gg 1$, however, the first viscous term is exponentially damped and the Langevin force determines the momentum,

$$\lim_{t\to\infty}\overline{p(t)^2} \to \frac{D}{\eta}$$

In this long-time limit, the kinetic energy

$$E_{\text{kinetic}} = \frac{\overline{p^2}}{2m} \to \frac{D}{2m\eta}.$$

与多普勒冷却极限的关系、



$F = -\underbrace{\alpha}_{\gamma} v$

$k_B T_D = \frac{D}{\alpha}$

$\frac{1}{2}\langle F(t)F(t')\rangle \sim (\hbar k)^2 R_{scatter} \sim (\hbar k)^2 \frac{\Gamma}{2}$

Δp^2

$\hbar k^2$

$T_D = \frac{\hbar k}{2}$