高等原子分子物理

自由电子发射 $e^- \to e^- + \gamma$ Xe: $I_p(Xe) = 12.1298eV, \hbar\omega = 2.33eV$, t $N = 6$但测出$N \gg 6$

切伦科夫辐射：u入射，散射角α

$$\cos\alpha = \frac{c}{\sqrt{\varepsilon_r}u}\left(1 - \frac{\varepsilon_r - 1}{2}\sqrt{1 - \frac{u^2}{c^2}}\frac{\hbar\omega}{mc^2}\right)$$

$\varepsilon_r = 1$: $\cos\alpha = \dfrac{c}{u} > 1$　不能发射　水：可以

Above Threshold Ionization(ATI)　阈上电离

能量 $U_p = \dfrac{e^2E_0^2}{4m\omega^2}a.u. = \dfrac{E_0^2}{4\omega^2}$　$U_p = 0.22a.u. = 5.99eV,\quad \Delta t \sim \dfrac{\hbar}{\Delta E} \sim 0.5a.u. \sim 12as$

HHG-ATI

t_0 出生时刻　$E(t) = E_0\sin\omega t,\quad v(t) = -\int_{t_0}^{t}E(t')\mathrm{d}t',\quad x(t) = \int_{t_0}^{t}v(t')\mathrm{d}t'$

$v(t) = \dfrac{E_0}{\omega}(\cos\omega t - \cos\omega t_0)$　第一项：oscillation　第二项：translation (drift)

驱动部分 $\dfrac{1}{2}mv_{drift}^2 = \dfrac{E_0^2}{2\omega^2}\cos^2\omega t_0 = 2U_p\cos^2\omega t \le 2U_p$

Recollision $x(t) = \int_{t_0}^{t}v(t')\mathrm{d}t' = -\dfrac{E_0}{\omega}(t - t_0)\cos\omega t_0 + \dfrac{E_0}{\omega^2}(\sin\omega t - \sin\omega t_0)$

回碰条件：$x(t_r) = 0 \implies (\omega t_r - \omega t_0)\cos\omega t_0 = \sin\omega t_r - \sin\omega t_0$

$t_0 \to t_r, t_r > t_0$ 讨论可知仅可$\dfrac{\pi}{2} \le \omega t_0 < \pi$或$\dfrac{3\pi}{2} \le \omega t_0 < 2\pi$

速度分解 $\begin{cases} v(t_r) = \dfrac{E}{\omega}(\cos\omega t - \cos\omega t_0) \\ v_{\parallel}(t_r) = v(t_r)\cos\theta \\ v_{\perp}(t_r) = v(t_r)\sin\theta \end{cases}$，之后

$$\begin{cases} v_{\parallel}(t) = v_{\parallel}(t_r) + \int_{t_r}^{t}a(t')\mathrm{d}t' = \dfrac{E}{\omega}(\cos\omega t_r - \cos\omega t_0)\cos\theta + \dfrac{E}{\omega}(\cos\omega t - \cos\omega t_r) \\ v_{\perp}(t) = v_{\perp}(t_r) = \dfrac{E}{\omega}(\cos\omega t_r - \cos\omega t_0)\sin\theta \end{cases}$$

电子动能 $E_k(t) = \frac{1}{2}(v_{//}^2(t) + v_{\perp}^2(t))$，即

$$\begin{aligned} E_k(t) = \frac{E_0^2}{2\omega^2}&[(\cos\omega t_r - \cos\omega t_0)^2 + (\cos\omega t - \cos\omega t_r)^2 \\ &+ 2(\cos\omega t_r - \cos\omega t_0)\cos\theta(\cos\omega t - \cos\omega t_r)] \end{aligned}$$

令$U_p = \frac{E_0^2}{4\omega^2}$，平均

$$\langle E_k\rangle = 2U_p[(\cos\omega t_r - \cos\omega t_0)^2 + \frac{1}{2} + \cos^2\omega t_0 - 2\cos\theta(\cos\omega t_r - \cos\omega t_0)\cos\omega t_r]$$

量子情形 $i\frac{\partial}{\partial t}\psi = \hat{H}\psi,\quad \hat{H} = \frac{1}{2}[p + A(t)]^2 - \varphi(x) = H_{pA}$

规范变换$\psi(x,t) \to e^{i\chi(x,t)}\psi(x,t), e = -1\quad H' = \frac{1}{2}[p + (A(t) + \nabla\chi)]^2 + (\varphi - \frac{\partial\chi}{\partial t})$

取$\chi=-A(t)x$，得到另一个规范 $H_{dE}=\frac{p^2}{2}-\varphi(x)+xE(t)$

两个规范下的波函数满足 $\psi_{pA}(t)=e^{-iA(t)x}\psi_{dE}(t)$

当$\varphi=0$时 $\vec{E}=-\frac{\partial\vec{A}}{\partial t}$， $\vec{v}(t)=\vec{p}+\vec{A}(t)=\vec{p}-\frac{\vec{E}}{\omega}\sin\omega t$

Volkov function

SFA: $i\frac{\partial}{\partial t}\psi=\frac{1}{2}(p+A(t))^2\psi,\quad \psi=N\varphi(t)e^{i\vec{p}\cdot\vec{r}}$

$\implies\ \varphi(t)=e^{-\frac{i}{2}\int^t[\vec{p}+\vec{A}(t')]\mathrm{d}t'}\ E(t)=E\cos\omega t,\vec{E}=-\frac{\partial\vec{A}}{\partial t}\implies\vec{A}(t)=-\frac{E}{\omega}\sin\omega t$

$$\psi_{PA}(\vec{r},t)=Ne^{i\vec{p}\cdot\vec{r}}e^{-i\left[\left(\frac{p^2}{2}+\frac{E^2}{4\omega^2}\right)t+\frac{\vec{p}\cdot\vec{E}}{\omega^2}-\frac{E^2}{4\omega^2}\frac{\sin2\omega t}{2\omega}\right]}$$

$$\psi_{dE}(\vec{r},t)=(2\pi)^{-\frac{3}{2}}e^{i\vec{p}\cdot\vec{r}}e^{-\frac{i}{2}\int^t v(t')^2\mathrm{d}t}=Ne^{i\vec{v}\cdot\vec{r}}e^{-i\left[\left(\frac{p^2}{2}+\frac{E^2}{4\omega^2}\right)t+\frac{\vec{p}\cdot\vec{E}}{\omega^2}-\frac{E^2}{4\omega^2}\frac{\sin2\omega t}{2\omega}\right]}$$

$a_p(t)=-i\int_{t_i}^t\mathrm{d}t'\left\langle\psi_f(p)\right|V_L(t')\left|\psi_i\right\rangle e^{i(E_f-E_i)t'}=-i\int_{t_i}^t\mathrm{d}t'\left\langle e^{i\vec{v}(t)\cdot\vec{r}}\right|V_L(t')\left|\psi_i\right\rangle e^{-\frac{i}{2}\int_{t'}^t v(\tau)^2\mathrm{d}\tau}e^{iI_pt'}$

鞍点近似 作用量$S(t,t')=-\frac{1}{2}\int_{t'}^t v(\tau)^2\mathrm{d}\tau+I_pt'$

$\frac{\partial S(t,t')}{\partial t'}=0\implies\frac{1}{2}v(t')^2+I_p=0,t'=t_0\quad v(t_0)=p-\dfrac{E}{\omega}\sin\omega t_0\overset{p=0}{=\!=\!=}-i\sqrt{2I_p}$

$t_0=it_0'',\quad\sinh\omega t_0''=\dfrac{\omega}{E}\sqrt{2I_p}=\gamma=\sqrt{\dfrac{I_p}{2U_p}}$ γ称为Keldysh参数

$x(t)=X(t)+\xi(t)$，其中$X(t)$慢，$\xi(t)$快 $\langle\xi(t)\rangle=0$ 有质动力势

$U(x)=U(X+\xi)\approx U(X)+\xi\frac{\mathrm{d}U}{\mathrm{d}X}+\cdots,\quad f(x,y)=f_0\cos\omega t=f(X+\xi,t)\approx f(X)+\xi\frac{\mathrm{d}f}{\mathrm{d}X}+\cdots$

$m\ddot{X}+m\ddot{\xi}=-\frac{\mathrm{d}U}{\mathrm{d}X}-\xi\frac{\mathrm{d}^2U}{\mathrm{d}X^2}+f(X,t)+\xi\frac{\mathrm{d}f}{\mathrm{d}X},\quad m\ddot{\xi}=f(X,t)+\xi\frac{\mathrm{d}f}{\mathrm{d}X}$

第二项快变，可略 $\ddot{\xi}\approx\omega^2\xi,\quad\xi=-\frac{f}{m\omega^2}$

运动方程取平均 $m\langle\ddot{X}\rangle=-\frac{\mathrm{d}U}{\mathrm{d}X}+\langle\xi\frac{\mathrm{d}f}{\mathrm{d}X}\rangle=-\frac{\mathrm{d}U}{\mathrm{d}X}-\frac{1}{m\omega^2}\langle f\frac{\mathrm{d}f}{\mathrm{d}X}\rangle=-\frac{\mathrm{d}(U+U_p)}{\mathrm{d}X}$

其中 $U_p=\frac{1}{2m\omega^2}\langle f^2\rangle$，对电磁场就是$U_p=\frac{E_0^2}{4m\omega^2}$

类比：参变共振的摆，振幅a $f_{eff}=-ma\omega^2\cos\omega t\sin\varphi$

有效势 $U_{eff}=U_p-mgl\cos\varphi=mgl[-\cos\varphi+\frac{a^2\omega^2}{4gl}\sin^2\varphi]$

在$\varphi=\pi$附近：$\varphi+\varepsilon\,U_{eff}(\varepsilon)\approx mgl[1-\frac{1}{2}(1-\frac{a^2\omega^2}{2gl})\varepsilon^2]$ $a\omega$较大时可以稳定平衡

在ψ_{dE}中的$e^{ix\sin2\omega t}$项，可利用$e^{ix\sin\gamma}=\sum_N J_N(x)e^{iN\gamma}$展开，对应等间隔的新的频率，即缀饰态 Dressed state

用虚时间表示的作用量 $S(0,t'=it_0'')=\frac{i}{2}\int_{t_0''}^0 v(i\tau)^2-iI_pt_0''$

代入$p=0$时$v(t)=-\frac{E}{\omega}\sin\omega t_0$后化简得到

$\mathrm{Im}S(0,t'=it_0'')=\frac{E^2}{4\omega^2}\frac{\gamma\sqrt{1+\gamma^2}}{\omega}-(\frac{I_p}{\omega}+\frac{E^2}{4\omega^2})\,\mathrm{arcsinh}\,\gamma$

再代入γ定义以及$U_p=\frac{E^2}{4\omega^2}$得到

$\mathrm{Im}S(0,t'=it_0'')=-\frac{I_p}{\omega}[(1+\frac{1}{2\gamma^2})\,\mathrm{arcsinh}\,\gamma-\frac{\sqrt{1+\gamma^2}}{2\gamma}]$

在$\gamma \ll 1$即$I_p \ll U_p$（强场）情况下$\mathrm{Im}S \approx -\frac{I_p}{\omega}\frac{4\gamma}{3} = -\frac{1}{3}2^{\frac{3}{2}}I_p^{\frac{3}{2}}E^{-1}$

相应跃迁概率幅$a_p \sim e^{\mathrm{Im}S(0,it_0'')} \sim e^{-\frac{(2I_p)^{\frac{3}{2}}}{3E}} \sim e^{-\frac{\sqrt{m_e}}{e\hbar}\frac{(2I_p)^{\frac{3}{2}}}{3E}} \sim e^{-\frac{1}{E}}$

在$\gamma \gg 1$即$I_p \gg U_p$（弱场）情况下$\mathrm{Im}S \approx -\frac{I_p}{\omega}\ln 2\gamma, \quad a_p \sim \frac{1}{(2\gamma)^{\frac{I_p}{\omega}}} \sim [\frac{E}{2\omega}\sqrt{2I_p}]^{\frac{I_p}{\omega}} \sim E^{\frac{I_p}{\omega}}$

单位制与量纲 a.u. $[\hbar],[m_e],[e],[4\pi\varepsilon_0]$ MKS $[M],[L],[T],[c]$

MKS到a.u.的转移矩阵 $A = \begin{pmatrix} 1 & 2 & -1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & -3 & 2 & 2 \end{pmatrix}$ 反过来 $B = A^{-1} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 2 & -1 & -2 & 1 \\ 2 & -1 & -4 & 2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

即$\begin{pmatrix} \ln[\hbar] \\ \ln[m_e] \\ \ln[e] \\ \ln[4\pi\varepsilon_0] \end{pmatrix} = A\begin{pmatrix} \ln[M] \\ \ln[L] \\ \ln[T] \\ \ln[c] \end{pmatrix}, \quad \begin{pmatrix} \ln[M] \\ \ln[L] \\ \ln[T] \\ \ln[c] \end{pmatrix} = B\begin{pmatrix} \ln[\hbar] \\ \ln[m_e] \\ \ln[e] \\ \ln[4\pi\varepsilon_0] \end{pmatrix}$

运用过来：$(\frac{I_p^{\frac{3}{2}}}{E})_{SI} = \frac{M^{\frac{3}{2}}L^3T^{-3}}{MLc^{-1}T^{-2}}(\frac{I_p^{\frac{3}{2}}}{E})_{a.u.} = \hbar m^{-\frac{3}{2}}(\frac{I_p^{\frac{3}{2}}}{E})_{a.u.}$

原子：跃迁、精细结构l,s、旋量表示、$SO(3,1)$旋量表示

应用：超冷原子和原子钟、GPS、合成规范场、自旋极化电子束流

双原子分子：分子振动与转动、不可约张量方法、Fano-Feshbach共振、Landau-Zener理论

多原子分子：振动与表示、fibre,bundle与不动点定理、j-invariant 魔群月光理论

含时微扰论 $i\hbar\frac{\partial\psi}{\partial t} = \hat{H}(t)\psi, \quad \hat{H}(t) = H_0 + H'(t)$

$\psi(x,t) = \sum_k c_k(t)e^{-\frac{iE_k^{(0)}t}{\hbar}}\psi_k^{(0)}(x) \quad H = -\vec{\mu}\cdot\vec{E}\frac{1}{2}(e^{i\omega t}+e^{-i\omega t})$

$c_m(t) = c_m(0) - \frac{i}{\hbar}\int_0^t e^{i\omega_{mn}t}\left\langle\psi_m^{(0)}\middle|\hat{H}'(t)\middle|\psi_n^{(0)}\right\rangle \mathrm{d}t$，代入计算得到

$c_m(t) = \delta_{mn} + \frac{i\vec{E}}{2\hbar}\cdot\left\langle\psi_m^{(0)}\middle|\vec{\mu}\middle|\psi_n^{(0)}\right\rangle[\frac{e^{i(\omega_{mn}+\omega)t}-1}{\omega_{mn}+\omega} + \frac{e^{i(\omega_{mn}-\omega)t}-1}{\omega_{mn}-\omega}]$

受激吸收（SA）：$\omega_{mn} = \omega, |m\rangle \to |n\rangle \quad \frac{\mathrm{d}N_n}{\mathrm{d}t} = B_{m\to n}N_m u(\nu_{mn})$

受激发射（SE）：$\omega_{mn} = -\omega, |n\rangle \to |m\rangle \quad \frac{\mathrm{d}N_n}{\mathrm{d}t} = -B_{n\to m}N_m u(\nu_{mn})$

自发辐射 $\frac{\mathrm{d}N_n}{\mathrm{d}t} = -A_{n\to m}N_n$

平衡时$\frac{\mathrm{d}N_n}{\mathrm{d}t} = 0$，得到$B_{n\to m} = B_{m\to n} = B$

以及$\frac{N_n}{N_m} = \frac{Bu(\nu_{mn})}{Bu(\nu_{mn})+A} = e^{-\frac{h\nu_{mn}}{k_bT}}, \quad u(\nu_{mn}) = \frac{8\pi h\nu_{mn}^3}{c^3}\frac{1}{e^{\frac{h\nu_{mn}}{k_BT}}-1}$

对比得到$A = \frac{8\pi h\nu_{mn}^3}{c^3}B$

光打入分子初态s，$l=1$，自旋（偏振）量子数$q \quad q=0 \to p_z, q=\pm1 \to p_x,p_y$

$SO(2): l=1, m_l=\pm1 \quad SO(3): l=1, m_l=\pm1,0$

要求矩阵元$\begin{pmatrix} l & 1 & l' \\ m_l & q & -m_l' \end{pmatrix} \neq 0$

$\vec{\mu} = -e\vec{r} = -er(\hat{i}\sin\theta\cos\varphi + \hat{j}\sin\theta\sin\varphi + \hat{k}\cos\theta)$

考察跃迁：$\langle\vec{\mu}\rangle = \langle\psi_{nlm_lm_s}|\vec{\mu}\,|n'l'm_l'm_s'\rangle$，计算得到

$$\langle\vec{\mu}\rangle = -e\int_0^\infty rR_{nl}(r)R_{n'l}(r)r\mathrm{d}r\int_0^\pi \sin\theta\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi Y_{lm}(\theta,\varphi)Y_{l'm'}(\theta,\varphi)\begin{pmatrix}\sin\theta\cos\varphi\\ \sin\theta\sin\varphi\\ \cos\theta\end{pmatrix}\delta_{m_3m_3'}$$

记矢量部分为$T_q^{(1)}, q=0,\pm1$　　选择定则$\forall\Delta n, \Delta m_s = 0, \Delta m_l = 0,\pm1, \Delta l = \pm1$

非零$\langle\mu_z\rangle$要求$\Delta l = \pm1, \Delta m_l = 0$，非零$\langle\mu_{x,y}\rangle$要求$\Delta l = \pm1, \Delta m_l = \pm1$

在$\langle\psi_f|\hat{O}\,|\psi_i\rangle$中，$|\psi_i(f)\rangle$是表示$\Gamma^{(i,f)}$的基函数，$\hat{O}$的表示为$\Gamma^{(o)}$

在矩阵元$\begin{pmatrix}l & 1 & l'\\ m_l & q & -m_l'\end{pmatrix}$，上半部分属于$SO(3)$，下半部分属于$SO(2)$

在σ^+光作用下，$l=1, m_j=-\frac{1}{2}, m_l=-1, m_s=\frac{1}{2}\to l=1, m_j=\frac{1}{2}, m_l=0, m_s=\frac{1}{2}$

即$|p^-\uparrow\rangle + |p^0\downarrow\rangle \to |p^0\uparrow\rangle$，亦即自旋翻转

He原子的Quantum defect theory

$H = H_0 + H', H' = \frac{e^2}{r_{12}}, H_0 = (-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{2e^2}{r_1}) + (-\frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{r_2})$

零阶 $H_0\psi_i^{(0)} = E_i^{(0)}\psi_i^{(0)}$,　$\psi_i^{(0)}(1,2) = \psi_1(1)\psi_2(2)$

其中 $\psi_1(1) = \sqrt{\frac{8}{\pi a_0^3}}e^{-\frac{2r_1}{a_0}}, \psi_2(2) = \sqrt{\frac{8}{\pi a_0^3}}e^{-\frac{2r_2}{a_0}}$，$E_0 = -\frac{4e^2}{a_0}$

一阶微扰 $\langle H'\rangle = \int\psi_0^{(0)}H'\psi_0^{(0)}\,\mathrm{d}\vec{r} = e^2\int_0^\infty\psi_1^2(1)[\frac{1}{r_1} - e^{-\frac{4r_1}{a_0}}(\frac{2}{a_0}+\frac{1}{r_1})]\,\mathrm{d}\vec{r}_1$

其中方括号内的项在$r_1\to0$趋于0，在$r_1\to\infty$趋于$\frac{e^2}{r_1}$

叠加上原子核构成了有效势

$$V_{eff}(r_1) = -\frac{2e^2}{r_1} + e^2\left[\frac{1}{r_1} - e^{-\frac{4r_1}{a_0}}(\frac{2}{a_0}+\frac{1}{r_1})\right]$$

$r_1\to0, V_{eff}(r_1)\to-\frac{2e^2}{r_1}, r_1\to\infty, V_{eff}(r_1)\to-\frac{e^2}{r_1}$

精确计算得到 $E_{He} = E_0 + \langle H'\rangle = \frac{5e^2}{4a_0} = -74.8eV$

$\uparrow\otimes\uparrow = \text{singlet}\otimes\text{triplet}$

$$|S\rangle_{asym} = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle),\quad |T\rangle_{sym} = \begin{cases}|\uparrow\uparrow\rangle\\ \downarrow\downarrow\\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\end{cases}$$

总波函数 $\psi_{tot} = \psi_{space}\psi_{spin}$，其单重态和三重态为

$$\begin{cases}\psi_{singlet} = |S\rangle_{asym}\otimes(\psi_1(r_1)\psi_2(r_2) + \psi_1(r_2)\psi_2(r_1))_{sym}\\ \psi_{triplet} = |T\rangle_{sym}\otimes(\psi_1(r_1)\psi_2(r_2) - \psi_1(r_2)\psi_2(r_1))_{asym}\end{cases}$$

x轴上的投影$|\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle), |\leftarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$

考虑$|T, s=1, m_s=0\rangle$的态：$|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle = (|\rightarrow\rightarrow\rangle - |\leftarrow\leftarrow\rangle)$

旋轨耦合 $|\vec{S}| = \frac{\hbar}{2}, \vec{\mu}_e = -g_e\frac{\mu_B\vec{S}}{\hbar}, g_e = 2(1+\frac{\alpha}{2\pi}+\cdots), \mu_B = \frac{e\hbar}{2m}$

电磁场$\vec{E}=\frac{Ze}{4\pi\varepsilon_0 r^2}\hat{r},\vec{B}=-\gamma\frac{\vec{v}\times\vec{E}}{c^2}$

哈密顿量 $\hat{H}_i^{so}=-\vec{\mu}_e\cdot\vec{B}=-\frac{g_e\mu_B\vec{S}}{\hbar}\frac{Ze}{4\pi\varepsilon_0 r}\frac{\vec{v}\times\hat{r}}{c^2}=2\xi(r)\frac{\vec{l}\cdot\vec{s}}{\hbar^2}$

考虑洛伦兹变换中$\vec{v}\to\vec{v}+\mathrm{d}\vec{v}$，矩阵变化$A(\vec{v}+\mathrm{d}\vec{v})=A(\vec{v})+\mathrm{d}\vec{v}\cdot\nabla_{\vec{v}}A(\vec{v})$

$t:\vec{x}'=A(\vec{\beta})\vec{x},\quad t+\delta t:\vec{x}''=A(\vec{\beta}+\delta\vec{\beta})\vec{x}$

$\vec{x}',\vec{x}''$的关系：$\vec{x}''=A_T\vec{x}'$, $A_T=A(\vec{\beta}+\delta\vec{\beta})A^{-1}(\vec{\beta})=A(\vec{\beta}+\delta\vec{\beta})A(-\vec{\beta})$

取$\vec{\beta}=(0,\beta,0,0),\delta\vec{\beta}=(0,\delta\beta_1,\delta\beta_2,0),A(\vec{\beta})=\begin{pmatrix}\gamma & -\gamma\beta & 0 & 0\\ -\gamma\beta & \gamma & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}$

对任意的$\vec{\beta}$，$A(\vec{\beta})=e^{\hat{\beta}\cdot\vec{K}\tanh^{-1}\beta}=\begin{pmatrix}\gamma & -\gamma\beta_1 & -\gamma\beta_2 & -\gamma\beta_3\\ -\gamma\beta_1 & \frac{1+(\gamma-1)\beta_1^2}{\beta^2} & \frac{(\gamma-1)\beta_1\beta_2}{\beta^2} & \frac{(\gamma-1)\beta_1\beta_3}{\beta^2}\\ -\gamma\beta_2 & -\frac{(\gamma-1)\beta_1\beta_2}{\beta^2} & \frac{1+(\gamma-1)\beta_2^2}{\beta^2} & \frac{(\gamma-1)\beta_2\beta_3}{\beta^2}\\ -\gamma\beta_3 & -\frac{(\gamma-1)\beta_1\beta_3}{\beta^2} & -\frac{(\gamma-1)\beta_2\beta_3}{\beta^2} & \frac{1+(\gamma-1)\beta_3^2}{\beta^2}\end{pmatrix}$

由此算出 $A_T=I-\frac{\gamma-1}{\beta^2}(\vec{\beta}\times\delta\vec{\beta})\cdot\vec{S}-(\gamma^2\delta\vec{\beta}_{\parallel}+\gamma\vec{\beta}_{\perp})\cdot\vec{K}=A(\Delta\beta)R(\Delta\Omega)$，

其中Boost部分 $A(\Delta\beta)=I-\Delta\vec{\beta}\cdot\vec{K}$，Rotation部分$R(\Delta\Omega)=I-\Delta\vec{\Omega}\cdot\vec{S}$，变化量

$$\begin{cases}\Delta\vec{\beta}=\gamma^2\delta\beta_{\parallel}+\gamma\delta\beta_{\perp}\\ \Delta\vec{\Omega}=\frac{\gamma-1}{\beta^2}(\vec{\beta}\times\delta\vec{\beta})=\frac{\gamma^2}{\gamma+1}(\vec{\beta}\times\delta\vec{\beta})\approx\frac{1}{2c^2}(\vec{v}\times\delta\vec{v})\end{cases}$$

根据转动系导数 $(\frac{\mathrm{d}G}{\mathrm{d}t})_{Rot}=(\frac{\mathrm{d}\vec{G}}{\mathrm{d}t})_{test}+\vec{\omega}_T\times\vec{G}$,

这里的角速度可看作$\vec{\omega}_T=\lim_{\delta t\to 0}\frac{\Delta\Omega}{\delta t}=\frac{\vec{v}\times\vec{a}}{2c^2}$，即Thomas进动

在量子情形中，$\frac{\mathrm{d}\vec{S}}{\mathrm{d}t}=(\frac{\mathrm{d}\vec{S}}{\mathrm{d}t})_{test}+\vec{\omega}_T\times\vec{S},\quad(\frac{\mathrm{d}\vec{S}}{\mathrm{d}t})_{test}=\vec{\mu}_e\times\vec{B}$，从哈密顿量即可得到

即 $\frac{\mathrm{d}\vec{S}}{\mathrm{d}t}=\vec{S}\times(\frac{g\mu_B}{\hbar}\vec{B}-\vec{\omega}_T)$，加速度$\vec{a}=\frac{e}{m}\vec{E}$，即$\vec{\omega}_T=-\frac{Ze^2}{4\pi\varepsilon_0 r^2}\frac{-1}{2m^2c^2}\vec{l}$

进而进动部分$\hat{H}_2^{so}=\vec{S}\cdot\vec{\omega}_T=-\frac{1}{2}(\frac{e\hbar}{mc})^2\frac{Z}{4\pi\varepsilon_0 r^3}\vec{l}\cdot\vec{s}=-\xi(r)\vec{l}\cdot\vec{s}$

总哈密顿量就是 $\hat{H}^{so}=\hat{H}_1^{so}+\hat{H}_2^{so}=\xi(r)\vec{l}\cdot\vec{s},\quad\xi(r)=O(\alpha^2)$

考虑飞机圆周运动　S:飞机系 S': Lab frame(LF)

考虑短时间：$\parallel$方向运动L,$\perp$方向运动W，S中$\varphi=\frac{W}{L}$，S'中$\varphi'=\frac{W}{\frac{L}{\gamma}}=\gamma\varphi$

加和就是$\sum\varphi'=2\pi\gamma$，多出来的部分就是进动角$\Delta\theta=2\pi(1-\gamma)$

进动角速度和角速度之比 $\frac{\omega_T}{\omega}=\frac{\Delta\theta}{2\pi}=1-\gamma=-\frac{1}{\sqrt{1-\beta^2}}+1\approx-\frac{1}{2}\beta^2$

由此得到$\omega_T=-\frac{1}{2}\beta^2\Omega=-\frac{1}{2c^2}v\cdot a=\frac{1}{2c^2}\vec{a}\times\vec{v}$

Rotation算符S和Boost算符K

转动：$S_1=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&1\\0&0&-1&0\end{pmatrix},\quad S_2=\begin{pmatrix}0&0&0&0\\0&0&0&-1\\0&0&0&0\\0&-1&0&0\end{pmatrix},\quad S_3=\begin{pmatrix}0&0&0&0\\0&0&-1&0\\0&1&0&0\\0&0&0&0\end{pmatrix}$

分别为绕x,y,z轴，如$e^{\theta S_1}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&\cos\theta&\sin\theta\\0&0&-\sin\theta&\cos\theta\end{pmatrix}$

Boost: $K_1=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix},\quad K_2=\begin{pmatrix}0&0&1&0\\0&0&0&0\\1&0&0&0\\0&0&0&0\end{pmatrix},\quad K_3=\begin{pmatrix}0&0&0&1\\0&0&0&0\\0&0&0&0\\1&0&0&0\end{pmatrix}$

分别为x,y,z轴上的boost，如$e^{-\zeta K_1}=\begin{pmatrix}\cosh\zeta&-\sinh\zeta&0&0\\-\sinh\zeta&\cosh\zeta&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}$

算符满足对易关系 $[S_i,S_j]=\varepsilon_{ijk}S_k,\quad [K_i,K_j]=-\varepsilon_{ijk}S_k,[S_i,K_j]=\varepsilon_{ijk}K_k$

Boost代数不封闭

由此可用Boost代数进行前面计算，一般洛伦兹矩阵$A(\hat\beta)=e^{\hat\beta\cdot K\varphi},\varphi=\tanh^{-1}\beta$

相应进动部分$A_T=A(\beta+\delta\beta)A(-\beta)=A(\hat\beta+\delta\hat\beta,\varphi+\delta\varphi)A(\hat\beta,-\varphi)=e^{(\hat\beta+\delta\hat\beta)\cdot K(\varphi+\delta\varphi)}e^{-\hat\beta\cdot K\varphi}$

利用CBH等式$e^Ae^B=e^{A+B+\frac12[A,B]+\frac1{12}([A,[A,B]]+[B,[B,A]])}$可以化简得到

$A_T=1+\hat\beta\cdot K\delta\varphi+\delta\hat\beta\cdot K\varphi-\frac12[\delta\hat\beta\cdot K,\beta\cdot K]\varphi^2$

利用$[K_r,K_s]=-\varepsilon_{rst}S_t$有$[\delta\hat\beta\cdot K,\hat\beta\cdot\hat K]=-(\delta\beta\times\beta)\cdot S$

进而$A_T=1+(\hat\beta\cdot K)\delta\varphi+(\delta\hat\beta\cdot K)\varphi-\frac12\varphi^2(\delta\hat\beta\times\beta)\cdot S$

与$\vec S$相关的代表rotation, 其转角为$\Omega_T\Delta t=\frac12\varphi^2(\delta\hat\beta\times\beta)=\frac12(\tanh^{-1}\beta)^2\frac{\delta\vec v\times\vec v}{c^2}$

因此角速度$\Omega_T=\frac12(\tanh^{-1}\beta)^2\frac{\vec a\times\vec v}{c}$

并旋量->并矢　$SO(3)$旋量表示->$SO(3,1)$旋量表示

$O(2)$ rotation: $R=\begin{pmatrix}\cos\theta&-\sin\theta\\\sin\theta&\cos\theta\end{pmatrix},\det|R|=1\quad \tau=\begin{pmatrix}\cos2\theta&\sin2\theta\\\sin2\theta&-\cos2\theta\end{pmatrix},\det|\tau|=1$

作$\mathbb{R}^3\to\mathbb{R}\times\mathbb{C}$的映射：$(x,y,z)\to(z,x+iy)$，并取旋量

$\tau=x\sigma_x+y\sigma_y+z\sigma_z=\begin{pmatrix}z&x-iy\\x+iy&-z\end{pmatrix}$

则$\hat e_x\to\sigma_x,\hat e_y\to\sigma_y,\hat e_z\to\sigma_z$

旋量τ把旋量$a=a_x\sigma_x+a_y\sigma_y+a_z\sigma_z$沿着与$(x,y,z)$垂直的面反射至$b=b_x\sigma_x+b_y\sigma_y+b_z\sigma_z$

给定$\hat n$，矢量可写为平行垂直分解$a=(a\cdot n)\hat n+(a-(a\cdot n)\hat n)=a_\parallel+a_\perp$，

沿与$\hat n$垂直的面反射为 $a'=-(a\cdot n)n+(a-(a\cdot n)n)=a-2(a\cdot n)n$（Euler-Rodrigues公式）

用σ作用有$\sigma\cdot a'=\sigma\cdot a-2(a\cdot n)(\sigma\cdot n)$

利用$(\sigma\cdot a)(\sigma\cdot b)=a\cdot b+i\sigma\cdot(a\times b)$有$a\cdot b=\frac{1}{2}\{(\sigma\cdot a),(\sigma\cdot b)\}$

进而$\sigma\cdot a'=-(\sigma\cdot n)(\sigma\cdot a)(\sigma\cdot n)$，即在垂直$\vec{n}$面的反射作用

连续两次反射：α,β，记$R=(\sigma\cdot\beta)(\sigma\cdot\alpha)$，则$\sigma a'=R(\sigma\cdot a)R$，$R$为Euler-Rodrigues矩阵

R的计算：设α,β夹角2φ且$\hat{n}$垂直α,β，则

$R=(\alpha\cdot\beta)-i(\alpha\times\beta)\cdot\sigma=\cos\frac{\varphi}{2}-i\sin\frac{\varphi}{2}\hat{n}\cdot\sigma=e^{i\frac{\varphi}{2}\hat{n}\cdot\sigma}$，且$R(4\pi,\hat{n})=1,R(2\pi,\hat{n})=1$

$SO(3)$: $a\to a'=\tilde{R}a,\qquad SU(2)$: $\sigma\cdot a\to\sigma\cdot a'=R(\sigma\cdot a)R$

$SU(2)$生成元：$X_{12}=-\frac{i}{2}\sigma_1\sigma_2,X_{23}=-\frac{i}{2}\sigma_2\sigma_3,X_{31}=-\frac{i}{2}\sigma_3\sigma_1$

考虑$SO(3,1)\to SL(2,\mathbb{C})$

从$\mathbb{R}^{3,1}\to(\mathbb{R}^2\times\mathbb{C})$: $(t,x,y,z)\to(t+z,t-z,x+iy)$即光锥坐标

取$Z=\begin{pmatrix}t+z & x-iy\\ x+iy & t-z\end{pmatrix}$，令$K^i=(\pm)\sigma_i,S^i=i\sigma_i$

对易关系$[K_i,K_j]=2\varepsilon_{ijk}S_k,[S_i,S_j]=-2\varepsilon_{ijk}S_k,[S_i,K_j]=-2\varepsilon_{ijk}K_k,[K_i,S_j]=-2\varepsilon_{ijk}K_k$

$R^{1,1}\times\mathbb{C}$空间的旋量基：$e,\sigma_1,\sigma_2,\sigma_3\quad Z=te+x\sigma_1+y\sigma_2+z\sigma_3$

Rotation $U_\theta=\begin{pmatrix}e^{-i\theta} & 0\\ 0 & e^{i\theta}\end{pmatrix},\quad U_\theta ZU_\theta^\dagger=\begin{pmatrix}t+z & e^{-2i\theta}(x-iy)\\ e^{2i\theta}(x+iy) & t-z\end{pmatrix}$，即
$x+iy\to e^{2i\theta}(x+iy)$

Boost $M_r=\begin{pmatrix}r & 0\\ 0 & r^{-1}\end{pmatrix},\quad M_rZM_r^\dagger=\begin{pmatrix}r^2(t+z) & x-iy\\ x+iy & r^{-2}(t-z)\end{pmatrix}$

相当于$\begin{cases}t'=\frac{1}{2}(r^2+r^{-2})t+\frac{1}{2}(r^2-r^{-2})z\\ z'=\frac{1}{2}(r^2-r^{-2})t+\frac{1}{2}(r^2+r^{-2})z\end{cases}$

令$r=e^{\frac{u}{z}}$，则相当于$\begin{cases}t'=\cosh u\,t+\sinh u\,z\\ z'=\sinh u\,t+\cosh u\,z\end{cases}$ 也可由$e^{u\sigma_x}=\begin{pmatrix}\cosh u & \sinh u\\ \sinh u & \cosh u\end{pmatrix}$得到

若用$J_i=-\frac{i}{2}S_i,K_i=-\frac{i}{2}\mathrm{K}_i$(前面的$K$)，$N_i^\pm=\frac{1}{2}(J_i\pm iK_i)$

对易关系$[N_i^-,N_j^-]=i\varepsilon_{ijk}N_k^-,[N_i^+,N_j^+]=i\varepsilon_{ijk}N_k^+,[N_i^+,N_j^-]=0$

即两部分对易关系独立，亦即$SO(3,1)\sim SU(2)_L\otimes SU(2)_R$，分解为Weyl spinor

$H=\sigma\cdot r=\begin{pmatrix}z & x-iy\\ x+iy & -z\end{pmatrix}=\begin{pmatrix}\xi_1 & \xi_2^*\\ \xi_2 & -\xi_1\end{pmatrix}$ 2D复空间$\xi=\begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix}$

令$S=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}=S^*$，构造对偶旋量$\chi=S\xi^*=\begin{pmatrix}-\xi_2^*\\ \xi_1^*\end{pmatrix}$

酉变换$U=\begin{pmatrix}a & b\\ -b^* & a^*\end{pmatrix}$，其满足$U=SU^*S^{-1}\implies US=SU^*$

在变换$\xi\to U\xi^*$下，$\chi\to(SU^*S^{-1})S\xi^*=U\chi$

定义$h=\xi\chi^\dagger=\begin{pmatrix}-\xi_1\xi_2 & \xi_1^2\\ -\xi_2^2 & \xi_1\xi_2\end{pmatrix}$，则$h\to UhU^\dagger$

令$h=H$得$\begin{cases}x=\frac{1}{2}(\xi_1^2-\xi_2^2)\\ y=\frac{i}{2}(\xi_1^2+\xi_2^2),\\ z=-\xi_1\xi_2\end{cases}\quad\begin{cases}\xi_1=\pm\sqrt{x-iy}\\ \xi_2=\pm\sqrt{-x-iy}\end{cases}$

$\begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix}$为旋量的2分量形式

$SO(3,1)=SU(2)_A\otimes SU(2)_B$ φ_A,φ_B分别为$SU(2)_A,SU(2)_B$的(Weyl)旋量

φ_A在$SU(2)_A$下变换，在$SU(2)_B$作用下不变，φ_B不同

$\begin{cases}\varphi_A\to e^{i\alpha_A N^+}\varphi_A; & \varphi_A\to e^{i\alpha_B N^-}\varphi_A=\varphi_A\\ \varphi_B\to e^{i\alpha_A N^+}\varphi_B=\varphi_B; & \varphi_B\to e^{i\alpha_B N^-}\varphi_B\end{cases}$

构造Lorentz $SO(3,1)$的Dirac旋量

$\begin{cases}e^{i\alpha_A N^+}\varphi_B=\sum_{n=0}^\infty\frac{1}{n!}(i\alpha_A N^+)^n\varphi_B=\varphi_B\implies N_i^+\varphi_B=0\implies S_i\varphi_B=-iK_i\varphi_B\\ e^{i\alpha_B N^-}\varphi_A=\sum_{n=0}^\infty\frac{1}{n!}(i\alpha_B N^-)^n\varphi_A=\varphi_A\implies N_i^-\varphi_A=0\implies S_i\varphi_A=iK_i\varphi_A\end{cases}$

φ_A: $J_i=-\frac{i}{2}S_i=\frac{\sigma_i}{2},\quad K_i=-iJ_i=-i\frac{\sigma_i}{2}$

φ_B: $J_i=\frac{\sigma_i}{2},\quad K_i=iJ_i=i\frac{\sigma_i}{2}$

Lorentz变换：$\varphi_A\to e^{i(\theta^i J_i+\varphi^i K_i)}\varphi_A=e^{\frac{i}{2}(\sigma\cdot\theta-i\sigma\cdot\varphi)}\varphi_A$

即$\begin{cases}\varphi_A\to e^{\frac{i}{2}\sigma\cdot(\theta-i\varphi)}\varphi_A\\ \varphi_A^\dagger\to\varphi_A^\dagger e^{-\frac{i}{2}\sigma\cdot(\theta+i\varphi)}\end{cases},\quad\begin{cases}\varphi_B\to e^{\frac{i}{2}\sigma\cdot(\theta+i\varphi)}\varphi_B\\ \varphi_B^\dagger\to\varphi_B^\dagger e^{-\frac{i}{2}\sigma\cdot(\theta-i\varphi)}\end{cases}$

一个静止的例子boost到动量p的态 $\varphi_{A,B}(0)\to\varphi_{A,B}(p)$

沿着$\hat{p}$作φ的boost变换 $\varphi=\varphi\hat{p}$

$$\begin{aligned}\varphi_A(p)&=e^{\sigma\cdot\frac{\varphi}{2}}\varphi_A(0)\\ &=\left[\sum_{n=0}^\infty\frac{1}{(2n)!}\left(\sigma\cdot\frac{\varphi}{2}\right)^{2n}+\sum_{n=0}^\infty\frac{1}{(2n+1)!}\left(\sigma\cdot\frac{\varphi}{2}\right)^{2n+1}\right]\varphi_A(0)\\ &=\left[\sum_{n=0}^\infty\frac{1}{(2n)!}\left(\frac{\varphi}{2}\right)^{n}+\sigma\cdot\hat{p}\sum_{n=0}^\infty\frac{1}{(2n+1)!}\left(\frac{\varphi}{2}\right)^{2n+1}\right]\varphi_A(0)\\ &=\left(\cosh\frac{\varphi}{2}+\sigma\cdot\hat{p}\sinh\frac{\varphi}{2}\right)\varphi_A(0)\end{aligned}$$

代入$\cosh\varphi=\gamma=\frac{E}{m}$，$|p|=\frac{p}{m\sqrt{\gamma^2-1}}$可得

$$\varphi_A=\frac{m(\gamma+1)+\sigma\cdot p}{\sqrt{2m^2(\gamma+1)}}\varphi_A(0)=\frac{E+m+\sigma\cdot p}{\sqrt{2m(E+m)}}\varphi_A(0)$$

同理

$$\varphi_B=\frac{E+m-\sigma\cdot p}{\sqrt{2m(E+m)}}\varphi_B(0)$$

静止系下$p=0,\varphi=0,\begin{cases}\varphi_A\to e^{\frac{i}{2}\sigma\cdot\theta}\varphi_A\\ \varphi_B=e^{\frac{i}{2}\sigma\cdot\theta}\varphi_B\end{cases}$

若$\varphi_A(0)=\varphi_B(0)$，则$\varphi_A(p)=\frac{E+m+\sigma\cdot p}{E+m-\sigma\cdot p}\varphi_B(p)$，即$\begin{cases}\varphi_A(p)=\frac{E+\sigma\cdot p}{m}\varphi_B(p)\\ \varphi_B(p)=\frac{E-\sigma\cdot p}{m}\varphi_A(p)\end{cases}$

亦即

$$\begin{pmatrix} -m & E+\sigma\cdot p \\ E-\sigma\cdot p & -m \end{pmatrix}\begin{pmatrix}\varphi_A(p)\\ \varphi_B(p)\end{pmatrix}=0$$

定义Dirac旋量(spinor) $\psi=\begin{pmatrix}\varphi_A\\ \varphi_B\end{pmatrix}$以及矩阵$\gamma^0=\begin{pmatrix}0 & I\\ I & 0\end{pmatrix},\gamma^i=\begin{pmatrix}0 & -\sigma_i\\ \sigma_i & 0\end{pmatrix}$

得到$(\gamma^\mu p_\mu-m)\psi(p)=0$

$E\sim i\frac{\partial}{\partial t},p\sim -i\nabla$，即有Dirac方程 $(i\partial\!\!\!/-m)\psi=0,\quad \partial\!\!\!/=\gamma^\mu\partial_\mu$

A^μ,A_μ分别为逆变，协变 $x^\mu=(t,\vec{x})\quad(x_\mu)=\langle x,e_\mu\rangle=x^\nu g_{\nu\mu}=(t,-\vec{x})$
$\partial^\mu=(\partial_0,-\nabla),\partial_\mu=(\partial_0,\nabla)$

逆变$A^\mu\to A'^\mu=\frac{\partial x'^\mu}{\partial x^\nu}A^\nu$ 协变$B_\mu\to B'_\mu=\frac{\partial x^\nu}{\partial x'^\mu}B_\mu$

引入$\alpha=\gamma^0\gamma^i=\begin{pmatrix}\sigma_i & 0\\ 0 & -\sigma_i\end{pmatrix},\beta=\gamma^0=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},$

哈密顿量$\hat{H}=c\alpha\cdot p+\beta mc^2,p=0$时$\hat{H}=\beta mc^2$

Weyl representation: $\alpha^W=\begin{pmatrix}\sigma & 0\\ 0 & -\sigma\end{pmatrix},\beta^W=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$

Dirac-Pauli representation $\alpha^{D-P}=\begin{pmatrix}0 & \sigma\\ \sigma & 0\end{pmatrix},\beta^{D-P}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

转换矩阵$W=\dfrac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}$，$\alpha_i^W=W^T\alpha_i^{D-P}W,\beta^W=W^T\beta^{D-P}W$

$i\hbar\frac{\partial}{\partial t}\psi=\hat{H}\psi,\hat{H}=c\alpha\cdot p+\beta mc^2$

$\dot{x}=c\alpha_x$，即$\hat{v}=c\hat{\alpha}$，$v=c$，但$\langle v\rangle_H=\frac{c^2p}{E}<c$

模式展开 $\psi(r,t)=\frac{1}{\hbar^{\frac{3}{2}}}\int[C^+(p)e^{-i\omega t}+C^-(p)e^{i\omega t}]e^{\frac{ip\cdot r}{\hbar}}\mathrm{d}^3p,\omega=\frac{E}{\hbar},E=\sqrt{c^2p^2+m^2c^4}$

其中$C^+(p)=a_1u_1+a_2u_2,\quad C^-(p)=a_3u_3+a_4u_4$

$$u_1=\begin{pmatrix}1\\0\\kp_3\\kp_+\end{pmatrix},\quad u_2=\begin{pmatrix}0\\1\\kp_-\\-kp_3\end{pmatrix},\quad u_3=\begin{pmatrix}-kp_3\\-kp_+\\1\\0\end{pmatrix},\quad u_4=\begin{pmatrix}-kp_-\\kp_3\\0\\1\end{pmatrix}$$

其中$k=\frac{c}{E+mc^2},p_\pm=p_1\pm ip_2$

平均速度$\langle v\rangle=\langle\dot{t}\rangle=c\langle\alpha\rangle=c\int(C^{+*}\alpha C^++C^{-*}\alpha C^-)\mathrm{d}^3p+2c\int\mathrm{Re}(C^{+*}\alpha C^-)e^{2i\omega t}\mathrm{d}^3p$

第二项代表量子拍（quantum beating）。利用$C^{\pm*}\alpha C^\pm=\pm\frac{cp}{E}C^{\pm*}C^\pm$可得

$$\langle\dot{r}\rangle=v+2c\int K(p)\sin(2\omega t+\varphi(p))\mathrm{d}^3p$$

其中$v=c\int\frac{p}{mc}(1+(\frac{p}{mc})^2)^{-\frac{1}{2}}(C^{+*}C^++C^{-*}C^-)\mathrm{d}^3p,$

$K(p)=|C^{-*}\alpha C^+|,\varphi(p)=\tan^{-1}\frac{\mathrm{Re}(C^{-*}\alpha C^+)}{\mathrm{Im}(C^{-*}\alpha C^+)}$

进而

$$\langle r\rangle = r^0 + vt - \bar{\lambda}\int K(p)\frac{1}{\sqrt{1+(\frac{p}{mc})^2}}\cos(2\omega t+\varphi(p))\mathrm{d}^3p,\quad \bar{\lambda}=\frac{\hbar}{mc}\sim 2pm$$

$t=0$时，$\psi(r,0)=\begin{pmatrix}1\\0\\0\\0\end{pmatrix}f(\frac{r}{r_0}),\quad f(\frac{r}{r_0})(\frac{2}{\pi r_0^3})^{\frac{3}{2}}e^{-\frac{r^2}{r_0^2}}$

而$C^+(p)=\frac{f(\frac{p}{\eta})}{1+k^2p^2}\begin{pmatrix}1\\0\\kp_3\\kp_+\end{pmatrix},\quad C^-(p)=\frac{f(\frac{p}{\eta})}{1+k^2p^2}\begin{pmatrix}k^2p^2\\0\\-kp_3\\-kp_+\end{pmatrix}$

利用$\psi(r,t=0)\sim\int[C^+(p)+C^-(p)]e^{\frac{ip\cdot r}{\hbar}}\mathrm{d}^3p$可知$\psi(p,t=0)\propto f(\frac{p}{\eta})\begin{pmatrix}1\\0\\0\\0\end{pmatrix}$

$t>0$，$\psi(r,t)=\frac{1}{\hbar^{\frac{3}{2}}}[\begin{pmatrix}1\\0\\kp_3\\kp_+\end{pmatrix}e^{-i\omega t}+\begin{pmatrix}k^2p^2\\0\\-kp_3\\-kp_+\end{pmatrix}e^{i\omega t}]\frac{f(\frac{p}{\eta})}{1+k^2p^2}e^{\frac{ip\cdot r}{\hbar}}\mathrm{d}^3p$

利用$r_0>\bar{\lambda},p\ll mc$可近似$k\approx\frac{1}{2mc}$，

$\psi(r,t)$的半经典轨道：近似有$K_1^{\alpha_1}(p)\approx\frac{f^2(\frac{p}{\eta})}{2mc}\sqrt{p_1^2+p_2^2},\quad K_2^{\alpha_2}(p)=K_1^{\alpha_1}(p),\quad K_3^{\alpha_3}=\frac{f^2(\frac{p}{\eta})}{2mc}p_3$

相应$\tan\varphi_i=\frac{\mathrm{Re}(C^{-*}\alpha_iC^+)}{\mathrm{Im}(C^{-*}\alpha_iC^+)}$，即$\begin{cases}\tan\varphi_1=-\frac{p_1}{p_2}\\ \tan\varphi_2=\frac{p_2}{p_1}\\ \tan\varphi_3=\infty\end{cases}$，即$\begin{cases}\varphi_1=\varphi+\pi\\ \varphi_2=\varphi\\ \varphi_3=\frac{\pi}{2}\end{cases}$

取球坐标$\begin{cases}p_1=p\sin\theta\cos\varphi\\ p_2=p\sin\theta\sin\varphi\\ p_3=p\cos\theta\end{cases}$，进而$K_1=K_2=\frac{f^2(\frac{p}{\eta})}{2mc}p\sin\theta,K_3=\frac{f^2(\frac{p}{\eta})}{2mc}p\cos\theta$

$\langle x_i\rangle$——电子颤动(jitter)的半经典轨道

积分得到 $\langle x_1\rangle=-I\int_0^{2\pi}\bar{\lambda}\sin(2\omega t+\varphi)\mathrm{d}\varphi$，$I=\frac{\bar{\lambda}}{32r_0}(\frac{2}{\pi})^{\frac{3}{2}}$，

里面关于φ的轨道 $\langle x_1\rangle_\varphi=-I\bar{\lambda}\sin(2\omega t+\varphi)$，同理$\langle x_2\rangle_\varphi=-I\bar{\lambda}\cos(2\omega t+\varphi)$

磁矩$\mu=\frac{1}{2c}\langle r\times j\rangle=\frac{e}{2c}\langle r\times\dot{r}\rangle$，

其中$\langle r\times\dot{r}\rangle=c\langle r\times\alpha\rangle\to i\hbar c\langle\nabla_p\times\alpha\rangle$，经过计算得到

$\langle r\times\dot{r}\rangle_1=\langle r\times\dot{r}\rangle_2=0,\quad\langle r\times\dot{r}\rangle_3=\frac{\hbar}{m}(1-\cos2\omega t)$，

从而$\mu_1=\mu_2=0,\quad\mu_3=\frac{e\hbar}{2mc}(1-\cos2\omega t)$

考虑绕核运动将会有修正效应，设电子速度$\vec{v}$，模型化为垂直原子平面的圆盘，进动角φ，圆周运动角ψ

实验室系(LF)下质点速度$\begin{cases}u_x=u_0\cos\psi\cos\varphi-v\\ u_y=u_0\cos\psi\sin\varphi\\ u_z=-u_0\sin\psi\end{cases}$，合起来$u^2=u_0^2+v^2-2vu_0\cos\psi\cos\varphi$

即$\gamma=\frac{1}{\sqrt{1-\frac{u^2}{c^2}}}\approx 1+\frac{u_0^2+v^2}{2c}-\frac{vu_0}{c^2}\cos\psi\cos\varphi$

实验系(LF)为S'，自旋系(SF)为S，关联$\begin{cases}x'=\gamma(x-vt)\\t'=\gamma(t-\frac{vx}{c^2})\\y'=y\\z'=z\end{cases}$，

在LF, $t'=0\implies$ SF, $t=\frac{vx}{c^2}, x=\frac{c^2}{v}t$且$x=r\sin(\omega t+\psi)\cos\varphi$

按ωt展开: $x=r\cos\varphi[\sin\psi+(\omega t)\cos\psi+O(\omega t)^2]$

代入$x=\frac{c^2}{v}t$得到$t=\frac{vr}{c^2}\cos\varphi\sin\psi$

从而$z'(t'=0)=z(t'=0)=z(t=\frac{vr}{c^2}\cos\varphi\sin\psi)=r\cos\left[\omega(\frac{vr}{c^2}\cos\varphi\sin\psi)+\psi\right]$

近似为$z'(t'=0)=r\cos\psi-\frac{vr^2}{c^2}\omega\cos\varphi\sin^2\psi$

质心位置　$\gamma_{dm}=\gamma(x',y',z')_{dm}$

$z'_{CM}=\langle\gamma z'\rangle_\psi$，近似计算得到$\gamma z'=-r\cos^2\psi\cos\varphi\frac{u_0 v}{c^2}-\frac{vr^2\omega}{c^2}\cos\varphi\sin^2\psi$

从而$z'_{CM}=-\frac{vr^2\omega}{c^2}\cos\varphi$

自旋 $S=|S|=|r\times p|=Mr^2\omega,\quad r^2\omega=\frac{S}{M}$，即$z'_{CM}=-\frac{vS}{Mc^2}\cos\varphi$

力$F=-M\frac{v^2}{R}$，自旋导数$\frac{\mathrm{d}S}{\mathrm{d}t}=(z\times F)_\perp=Fz\cos\varphi=\frac{v^3S}{Rc}\cos^2\varphi$

进动角速度$\frac{\mathrm{d}\varphi}{\mathrm{d}t}=\frac{1}{S}\frac{\mathrm{d}S}{\mathrm{d}t}=\frac{v^3}{Rc^2}\cos^2\varphi$

令$\Omega=\frac{v}{R},\beta=\frac{v}{c}$则$\frac{\mathrm{d}\varphi}{\mathrm{d}t}=\Omega\beta^2\cos^2\varphi$，均值$\langle\frac{\mathrm{d}\varphi}{\mathrm{d}t}\rangle_\varphi=\frac{1}{2}\Omega\beta^2=\Omega_T$

加速度$a=-v\Omega$，故$\Omega_T=-\frac{1}{2}\frac{a\cdot v}{c^2},\frac{\Omega_T}{\Omega}=\frac{1}{2}\beta^2$,

考虑多电子原子，$\hat{H}=\sum_i(-\frac{\hbar^2}{2m}\nabla_i^2-\frac{Ze^2}{r_i})+\sum_{ij}\frac{e^2}{r_{ij}}+\sum_i\zeta(r_i)\hat{l}_i\cdot\hat{s}_i$

$\zeta(r)\propto\frac{1}{2}\frac{Z\alpha^2}{r^3}$，$Z\uparrow,r\downarrow\implies\zeta\uparrow$，自旋轨道耦合$E_{SOC}\uparrow$

例：$^3D_1,|L=2,S=1,J=1,M_J=0\rangle$

最高权态出发 $|L=2,S=1,J=3,M_J=3\rangle=|L=2,S=1,M_L=2,M_S=1\rangle$

$\hat{J}_-|2133\rangle(LSJM_J)=(\hat{L}_-+\hat{S}_-)|2121\rangle(LSM_LM_S)$

利用$J_\pm|JM_j\rangle=\sqrt{J(J+1)-M_J(M_J\pm1)}|JM_J\pm1\rangle$得

$|2132\rangle=\frac{2}{\sqrt{6}}|2111\rangle+\frac{1}{\sqrt{3}}|2120\rangle$

J降1：$|2122\rangle=a|2111\rangle+b|2120\rangle$

要求$\langle 2122|2132\rangle=0$与归一$\implies|2122\rangle=-\frac{1}{\sqrt{3}}|2111\rangle+\sqrt{\frac{2}{3}}|2120\rangle$

同理$|2111\rangle=-\frac{1}{\sqrt{10}}|2101\rangle+\sqrt{\frac{3}{10}}|2110\rangle-\sqrt{\frac{3}{5}}|212-1\rangle$

$|2110\rangle=\sqrt{\frac{3}{10}}|21-11\rangle-\sqrt{\frac{2}{5}}|2100\rangle+\sqrt{\frac{3}{10}}|211-1\rangle$

系数记为C-G系数$\begin{pmatrix}2&1&1\\-1&1&0\end{pmatrix}$等，即$\begin{pmatrix}j_1&j_2&J\\m_1&m_2&M\end{pmatrix}$

亦即$|lsjm_j\rangle = \sum_{m_l m_s} |lsm_l m_s\rangle \langle lsm_l m_s|lsjm_j\rangle$，$\langle lsm_l m_s|lsjm_j\rangle$为C-G系数

3Γ Coefficient (Fano V Coefficient)

$\Gamma_1 \otimes \Gamma_2 = \sum_i c_i \Gamma_i \qquad |\Gamma_1, \Gamma_2, \Gamma, M\rangle = \sum_{M_1 M_2} \langle \Gamma_1 M_1 \Gamma_2 M_2|\Gamma M\rangle |\Gamma_1 M_1\rangle |\Gamma_2 M_2\rangle$

归一关系 $\sum_{M_1 M_2} \langle \Gamma_1 M_1 \Gamma_2 M_2|\Gamma M\rangle \langle \Gamma_1 M_1 \Gamma_2 M_2|\Gamma' M'\rangle = \delta_{\Gamma'\Gamma}\delta_{M'M}$

交换关系 $\begin{pmatrix} \Gamma_2 & \Gamma_1 & \Gamma_3 \\ M_2 & M_1 & M_3 \end{pmatrix} = (-)^{\Gamma_1+\Gamma_2+\Gamma_3} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ M_1 & M_2 & M_3 \end{pmatrix}$

Wigner-Eckart定理 $\langle \Gamma_1 M_1|\hat{O}^{\Gamma_2}_{M_2}|\Gamma_3 M_3\rangle \propto \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma_3 \\ M_1 & M_2 & M_3 \end{pmatrix} \langle \Gamma_1||O^{\Gamma_2}||\Gamma_3\rangle$

自旋极化的电子源

$\psi_K^{p-e,k_e} = \sum_{p^\alpha, R_N^\alpha} c_{p\alpha}(R_N^\alpha)\varphi_{p^\alpha}^{AO}(r_e - R_N^\alpha) \sim \sum_{p^\alpha, R_N^\alpha} e^{iK\cdot R_N^\alpha}\tilde{c}_p(R_N^\alpha)\varphi_{p^\alpha}^{AO}(r_\alpha - R_N^\alpha)$

$K = 0$时 $\varphi_0^{p-e,k_e}(r_e) = \sum_{p^\alpha, R_N^\alpha} \tilde{c}_p(R_N^\alpha)\varphi_{p^\alpha}^{AO}(r_e - R_N^\alpha)$

苯分子 C_6对称群 $|\psi_k\rangle \sim \frac{1}{\sqrt{n}}(|v_1\rangle + e^{i\frac{k}{n}2\pi}|v_2\rangle + \cdots e^{i\frac{k}{n}(n-1)2\pi}|v_n\rangle)$

$$n = 6{:}\, H = \begin{pmatrix} \alpha & \beta & 0 & 0 & 0 & \beta \\ \beta & \alpha & \beta & 0 & 0 & 0 \\ 0 & \beta & \alpha & \beta & 0 & 0 \\ 0 & 0 & \beta & \alpha & \beta & 0 \\ 0 & 0 & 0 & \beta & \alpha & \beta \\ \beta & 0 & 0 & 0 & \beta & \alpha \end{pmatrix} \varepsilon_k = \alpha + 2\beta\cos\frac{\pi}{3}k\,\beta < 0$$

$\alpha + 2\beta$成键 $\quad \alpha - 2\beta$反键

$S_{1/2}{:}\, l = 0, s = \frac{1}{2}, j = \frac{1}{2}$

$\left|\frac{1}{2}\frac{1}{2}\right\rangle_{j,m_j} = \left|0\frac{1}{2}\frac{1}{2}\frac{1}{2}\right\rangle_{l,s,j,m_j} = \left|0, \frac{1}{2}, 0, \frac{1}{2}\right\rangle_{l,s,m_l,m_s} = |s\uparrow\rangle$

$\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \left|0, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right\rangle = \left|0, \frac{1}{2}, 0, -\frac{1}{2}\right\rangle = |s,\downarrow\rangle$

$P_{3/2}{:}\, l = 1, s = \frac{1}{2}, j = \frac{3}{2}$

$\left|\frac{3}{2}\frac{3}{2}\right\rangle = \left|1\frac{1}{2}1\frac{1}{2}\right\rangle = |P^+\uparrow\rangle$

$\left|\frac{3}{2}\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left|1\frac{1}{2}1 - \frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|1\frac{1}{2}0\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}|P^+\downarrow\rangle - \sqrt{\frac{2}{3}}|P^0\uparrow\rangle$

$\left|\frac{3}{2}, -\frac{1}{2}\right\rangle = -\frac{1}{\sqrt{3}}\left|1, \frac{1}{2}, -1, \frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|1, \frac{1}{2}, 0, -\frac{1}{2}\right\rangle = -\frac{1}{\sqrt{3}}|P^-\uparrow\rangle - \sqrt{\frac{2}{3}}|P^0\downarrow\rangle$

$\left|\frac{3}{2}, -\frac{3}{2}\right\rangle = -\left|1, \frac{1}{2}, -1, -\frac{1}{2}\right\rangle = |P^-\downarrow\rangle$

$P_{1/2}{:}$

$\left|\frac{1}{2}\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1, \frac{1}{2}, 1, -\frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\left|1, \frac{1}{2}, 0, \frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}|p^+\downarrow\rangle + \sqrt{\frac{1}{3}}|p^0\uparrow\rangle$

$\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1, \frac{1}{2}, -1, \frac{1}{2}\right\rangle - \sqrt{\frac{1}{3}}\left|1, \frac{1}{2}, 0, -\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}|p^-\uparrow\rangle - \sqrt{\frac{1}{3}}|p^0\downarrow\rangle$

Sisyphus劈裂

相向电场$\vec{e} = \hat{e}_x, \vec{e}' = \hat{e}_y, E_0 = E_0'$

总电场 $E(z,t)=E_0\cos(\omega t-kz)\vec{e}+E_0'\cos(\omega t+kz)=E^+(z)e^{-i\omega t}+E^-(z)e^{i\omega t}$

其中 $E^+(z)=\frac{1}{2}(E_0\hat{e}_xe^{ikz}+E_0\hat{e}_ye^{-ikz})=\frac{E_0}{\sqrt{2}}(\vec{\varepsilon}_1\cos kz-i\vec{\varepsilon}_2\sin kz)$

$\vec{\varepsilon}_1=\frac{\hat{e}_x+\hat{e}_y}{\sqrt{2}},\quad \vec{\varepsilon}_2=\frac{\hat{e}_y-\hat{e}_x}{\sqrt{2}}$

$z=0$: $E^+(z)\propto\frac{\hat{e}_x+\hat{e}_y}{\sqrt{2}}$，线偏$\vec{\varepsilon}_1$

$z=\frac{\lambda}{8}:E^+(z)\propto\vec{\varepsilon}_1-i\varepsilon_2,\sigma^-$圆偏

$z=\frac{\lambda}{4}:E^+(z)\propto-i\vec{\varepsilon}_2$，线偏$-\vec{\varepsilon}_2$

$z=\frac{3\lambda}{8}:E^+(z)\propto\vec{\varepsilon}_1+i\vec{\varepsilon}_2,\sigma^+$圆偏

$z=\frac{\lambda}{2}$: $E^+(z)\propto-\vec{\varepsilon}_1$，线偏$-\vec{\varepsilon}_1$

Na: ${}^2S_{1/2}\leftrightarrow\ {}^2P_{3/2}$，记为$g,e$　偏振梯度

$\left|g_{-\frac{1}{2}}\right\rangle\xrightarrow{\sigma_+}\left|e_{+\frac{1}{2}}\right\rangle\propto(\frac{1}{\sqrt{3}})^2\quad\left|g_{\frac{1}{2}}\right\rangle\xrightarrow{\sigma_+}\left|e_{\frac{3}{2}}\right\rangle\propto 1$

$\delta E\propto|\langle f|H|i\rangle|^2\quad P_{21}=\langle 2|H|1\rangle,\Omega=P_{21}\frac{E_0}{\hbar}$

$$\begin{cases}i\frac{\mathrm{d}c_1}{\mathrm{d}t}=-\frac{\Omega}{2}e^{i\delta t}c_2\\ i\frac{\mathrm{d}c_2}{\mathrm{d}t}=-\frac{\Omega}{2}e^{-i\delta t}c_1\end{cases}\quad\begin{pmatrix}c_1'=c_1\\ c_2'=c_2e^{i\delta t}\end{pmatrix}\implies\begin{cases}i\hbar\frac{\mathrm{d}c_1'}{\mathrm{d}t}=-\frac{\hbar\Omega}{2}c_2'\\ i\hbar\frac{\mathrm{d}c_2'}{\mathrm{d}t}=-\frac{\hbar\Omega}{2}c_1'+\hbar\delta c_2'\end{cases}$$

即$i\hbar\begin{pmatrix}c_1'\\ c_2'\end{pmatrix}=H\begin{pmatrix}c_1'\\ c_2'\end{pmatrix},\quad H=\begin{pmatrix}0&-\frac{\hbar\Omega}{2}\\ -\frac{\hbar\Omega}{2}&\hbar\delta\end{pmatrix}$

$E_{12}=\frac{\hbar(\delta\pm\sqrt{\delta^2+\Omega^2})}{2}\ \Omega\ll\delta$时$\begin{cases}E_1=-\frac{\hbar}{4}\frac{\Omega^2}{\delta}\\ E_2=\hbar\delta+\frac{\hbar}{4}\frac{\Omega^2}{\delta}\end{cases}$

即$\delta E_1=-\frac{\hbar}{4}\frac{\Omega^2}{\delta},\quad\delta E_2=+\frac{\hbar}{4}\frac{\Omega^2}{\delta}$

平均力 $\vec{f}=\frac{\langle\Delta\vec{p}\rangle}{\Delta t}=\frac{1}{\Delta t}\langle\hbar\vec{k}(N_+-N_-)+\sum_{sp}\hbar\vec{k}_{sp}\rangle=\hbar\vec{k}\frac{\langle N_+\rangle-\langle N_-\rangle}{\Delta t}$

由于$\langle N_+\rangle-\langle N_-\rangle=n_1\Gamma_{12}\Delta t-n_2\Gamma_{21}\Delta t$，且由平衡关系$n_1\Gamma_{12}=n_2\Gamma_{21}+n_2\Gamma_{sp}$

可知$\langle N_+\rangle-\langle N_-\rangle=n_2\Gamma_{sp}\Delta t$，即 $\vec{f}=\hbar\vec{k}n_2\Gamma_{sp}$

$H=H_0+H_1,\quad H_0=\hbar\omega_1|1\rangle\langle 1|+\hbar\omega_2|2\rangle\langle 2|,\quad H_1=-\frac{1}{2}\vec{\mu}_0\cdot\vec{E}e^{i\omega t}|1\rangle\langle 2|$

由刘维尔方程知

$\dot{\rho}_{11}=\frac{1}{i\hbar}[(H_0+H_1),\rho]_{11}-\frac{1}{T_{11}}(\rho_{11}-\rho_{11}^0)$

$\dot{\rho}_{22}=\frac{1}{i\hbar}[(H_0+H_1),\rho]_{22}-\frac{1}{T_{22}}(\rho_{22}-\rho_{22}^0)$

$\dot{\rho}_{12}=\frac{1}{i\hbar}[(H_0+H_1),\rho]_{12}-\frac{\rho_{12}}{T_{12}}$

$\dot{\rho}_{21}=\frac{1}{i\hbar}[(H_0+H_1),\rho]_{21}-\frac{\rho_{21}}{T_{21}}$

其中$T_{11}=T_{22}=T_1=\frac{1}{\Gamma},T_{12}=T_{21}=T_2=\frac{2}{\Gamma},\Gamma=\Gamma_{sp}$

无哈密顿量时 $\dot{\rho}_{ij}=-\frac{\rho_{ij}-\rho_{ij}^0}{T_{ij}}$，即$\rho_{22}\sim e^{-\Gamma t},c_2\sim e^{-\frac{\Gamma}{2}t},c_1\sim 1,\rho_{12}\sim e^{-\frac{\Gamma}{2}t}$

计算哈密顿量项：$[H_0,\rho]_{ij}=(E_i-E_j)\rho_{ij}$

$[H_1,\rho]_{11}=(H_1)_{12}\rho_{21}-\rho_{12}(H)_{21}=(H_1)_{12}\rho_{21}-\rho_{21}^*(H_1)_{12}^*=2i\,\mathrm{Im}[(H_1)_{12}\rho_{21}]=-[H_1,\rho]_{22}$

$[H_1,\rho]_{12}=(H_1)_{11}\rho_{12}+(H_1)_{12}\rho_{12}-\rho_{11}(H_1)_{12}-\rho_{12}(H_1)_{22}=(H_1)_{12}(\rho_{22}-\rho_{11})=-[H_1,\rho]_{21}^*$

其中用到了$(H_1)_{ii}=0$，令$\rho_{12}=\bar\rho_{12}e^{i\omega t},\rho_{21}=\bar\rho_{21}e^{-i\omega t}$

则$2\,\mathrm{Im}[(H_1)_{12}\rho_{21}]=\frac{i}{2}\vec\mu_{12}\cdot\vec E(\bar\rho_{21}-\bar\rho_{12})$

初始 $\rho_{11}(0)=1,\rho_{22}(0)=0$，且$k_BT\ll E_2-E_1$，则

$$\begin{cases}\dot\rho_{11}=i\frac{\vec\mu_{12}\cdot\vec E}{2\hbar}(\bar\rho_{21}-\bar\rho_{12})-\Gamma(\rho_{11}-1)\\ \dot\rho_{22}=-i\frac{\vec\mu_{12}\cdot\vec E}{2\hbar}(\bar\rho_{21}-\bar\rho_{12})-\Gamma\rho_{22}\\ \dot\rho_{12}=i(\omega_0-\omega)\bar\rho_{12}+i\frac{\vec\mu_{12}\cdot\vec E}{2\hbar}(\rho_{22}-\rho_{11})-\frac{\Gamma}{2}\bar\rho_{12}\\ \dot\rho_{21}=-i(\omega_0-\omega)\bar\rho_{21}-i\frac{\vec\mu_{12}\cdot\vec E}{2\hbar}(\rho_{22}-\rho_{11})-\frac{\Gamma}{2}\bar\rho_{21}\end{cases}$$

其中$\omega_0\approx(\omega_2-\omega_1)+k\hat e_{\vec k}\cdot\vec v=\omega_{21}+k\hat e_{\vec k}\cdot\vec v$

考虑稳态并令$n_2=\rho_{22}$得

$$\begin{cases}\Gamma n_2=-i\frac{\vec\mu\cdot\vec E}{2\hbar}(\bar\rho_{21}-\bar\rho_{12})\\ -i(\omega_0-\omega)\bar\rho_{12}+i\frac{\vec\mu\cdot\vec E}{2\hbar}(2n_2-1)=\frac{\Gamma\bar\rho_{12}}{2}\\ -i(\omega_0-\omega)\bar\rho_{21}-i\frac{\vec\mu\cdot\vec E}{2\hbar}(2n_2-1)=\frac{\Gamma\bar\rho_{21}}{2}\end{cases}$$

解出

$$n_2=\frac{(\frac{\vec\mu\cdot\vec E}{2\hbar})^2}{[(\omega_0-\omega)^2+(\frac{\Gamma}{2})^2]+2(\frac{\vec\mu\cdot\vec E}{2\hbar})^2}$$

令$\Delta=\omega-\omega_{21}$得

$$n_2=\frac{(\frac{\vec\mu\cdot\vec E}{2\hbar})^2}{(\Delta-k\hat e_k\cdot\vec v)^2+2(\frac{\vec\mu\cdot\vec E}{2\hbar})^2+(\frac{\Gamma}{2})^2}$$

相应

$$\vec f=\hbar\vec k\Gamma_{sp}n_2=\frac{\hbar\vec k\Gamma(\frac{\vec\mu\cdot\vec E}{2\hbar})^2}{(\Delta-k\hat e_k\cdot\vec v)^2+2(\frac{\vec\mu\cdot\vec E}{2\hbar})^2+(\frac{\Gamma}{2})^2}$$

考虑正反两方向知

$$\vec f_s=\vec f_{\vec k}+\vec f_{-\vec k}=\hbar\vec k\Gamma\left[\frac{(\frac{\vec\mu\cdot\vec E}{\hbar\Gamma})^2}{\frac{(\Delta-k\hat e_{\vec k}\cdot\vec v)^2}{(\frac{\Gamma}{2})^2}+2(\frac{\vec\mu\cdot\vec E}{\hbar\Gamma})^2+1}-\frac{(\frac{\vec\mu\cdot\vec E}{\hbar\Gamma})^2}{\frac{(\Delta+k\hat e_{\vec k}\cdot\vec v)^2}{(\frac{\Gamma}{2})^2}+2(\frac{\vec\mu\cdot\vec E}{\hbar\Gamma})^2+1}\right]$$

$kv\ll\Delta$时

$$\vec f=\left\{\frac{\delta\hbar\vec k}{\Gamma}\frac{\Delta(\frac{\mu_{12}E}{\hbar\Gamma})^2\vec k}{[\frac{\Delta^2}{(\frac{\Gamma}{2})^2}+2(\frac{\vec\mu\cdot\vec E}{\hbar\Gamma})^2+1]^2}\right\}\cdot\vec v\propto\Delta\vec k\vec k\cdot\vec v$$

原子钟 GPS系统 $(x-A_i)^2+(y-B_i)^2+(z-C_i)^2-[c(T_i-d)]^2=0$

接收$\tilde{T}_0 = T_0 + \frac{D}{c}, \quad D' = c(T_1 - T_0')$

Cs钟 $N = 10^6, T = 0.9s \quad \Delta|\omega - \omega_0| = \frac{1}{2T\sqrt{N}} = 5.6 \times 10^{-4} Hz,$
$\omega_0 \sim 2\pi \times 9.2GHz, \frac{\Delta\omega}{\omega} \sim 10^{-14}, \Delta T \sim 8.6 \times 10^{-10}s, c\Delta T = 0.25m$

以g下降的电梯中，光下落H，光源$v = gt = g\frac{H}{c} \qquad \omega_B = \omega_A(1 + \frac{v}{c}) = \omega_A(1 + \frac{gH}{c^2})$

原子跃迁装置Cs, Rb $\Longrightarrow$ 频率发生器(转换) $\Longrightarrow$ 晶振 $\Longrightarrow$ 标准频率输出

跃迁过程$|1\rangle \to |2\rangle, \frac{N_2 - N_1}{N} \propto f(|\omega - \omega_0|\frac{T}{2})$

Cs: $S_e = \frac{1}{2}, S_n = I = \frac{7}{2}, J = S = \frac{1}{2}, F = I + J = 4, 3$

在$1m$尺度上下振动，周期$T = 2\sqrt{\frac{2H}{g}} = 0.9s$，频率劈裂$\omega = \omega_0 \pm \frac{\pi}{2T}, \Delta\omega = 1.7Hz$

测N次: $\begin{cases} T(F=4) & p \\ F(F=3) & 1-p=q \end{cases} \qquad \langle T \rangle = Np, \Delta^2 = Npq, \Delta = \sqrt{Npq}$

设$\varphi = (\omega - \omega_0)\frac{T}{2}$，则$\langle N_1 \rangle = N\sin^2\varphi, \langle N_2 \rangle = N\cos^2\varphi$

则$\Delta N_1 = \Delta N_2 = \sqrt{N}|\sin\varphi\cos\varphi|, \frac{\Delta(N_2 - N_1)}{N} = \frac{1}{\sqrt{N}}|\sin 2\varphi|$

同时$\frac{N_2 - N_1}{N} = \cos 2\varphi, \quad \frac{\Delta(N_2 - N_1)}{N} = 2|\sin 2\varphi|\Delta\varphi$

由以上两种等价可知$\Delta\varphi = \frac{1}{2\sqrt{N}} \Longrightarrow \Delta|\omega - \omega_0| = \frac{1}{2T\sqrt{N}}$

令$|1\rangle, |2\rangle = \{|F = 3, 4\rangle\}$，量子态$|\psi(t)\rangle = \alpha\,|1\rangle + \beta\,|2\rangle = \cos\frac{\theta}{2}|1\rangle + e^{i\varphi}\sin\frac{\theta}{2}|2\rangle$

在电场$E = E_0\cos(\omega t + \varphi)$

$$\begin{cases} \alpha(t+\varepsilon) = e^{i\frac{\delta t}{2}}\left[\alpha(t)\left(\cos\frac{\Omega_R\varepsilon}{2} + i\cos\theta\sin\frac{\Omega_R\varepsilon}{2}\right) + \beta(t)e^{i(\delta t + \varphi)}\left(-i\sin\theta\sin\frac{\Omega_R\varepsilon}{2}\right)\right] \\ \beta(t+\varepsilon) = e^{-i\frac{\delta t}{2}}\left[\alpha(t)e^{-i(\delta t + \varphi)}\left(-i\sin\theta\sin\frac{\Omega_R\varepsilon}{2}\right) + \beta(t)\left(\cos\frac{\Omega_R\varepsilon}{2} - i\cos\theta\sin\frac{\Omega_R\varepsilon}{2}\right)\right] \end{cases}$$

其中$\sin\theta = \frac{\Omega}{\Omega_R}, \cos\theta = -\frac{\delta}{\Omega_R}$，失谐$\delta = \omega - \omega_0$，拉比频率$\Omega_R = \sqrt{\Omega^2 + \delta^2}, \Omega = \frac{\langle 2|\mu \cdot E|1\rangle}{\hbar}$
$\Omega_R \sim MHz - GHz$

在$\delta = 0$时，$\sin\theta = 1, \cos\theta = 1,$ $\begin{cases} \alpha(t+\varepsilon) = \alpha(t)\cos\frac{\Omega\varepsilon}{2} + \beta(t)e^{i\varphi}(-i\sin\frac{\Omega\varepsilon}{2}) \\ \beta(t+\varepsilon) = \alpha(t)e^{-i\varphi}(-i\sin\frac{\Omega\varepsilon}{2}) + \beta(t)\cos\frac{\Omega\varepsilon}{2} \end{cases}$

取$\Omega\varepsilon = \pi$即π—操作: $\alpha(t+\varepsilon) = -i\beta e^{i\varphi}, \beta(t+\varepsilon) = -i\alpha e^{i\varphi}$，即$O_\pi = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$

同理$O_{\frac{\pi}{2}} = \dfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & -ie^{i\varphi} \\ -ie^{-i\varphi} & 1 \end{pmatrix}$

对于$\delta = 0$的情况，取$\alpha(0) = 1, \beta(0) = 0, \Omega_R\varepsilon = \frac{\pi}{2},$ $\begin{cases} \alpha(\varepsilon) = e^{i\frac{\delta\varepsilon}{2}}\frac{1 + i\cos\theta}{\sqrt{2}} \\ \beta(\varepsilon) = -e^{-i\frac{\delta\varepsilon}{2}}e^{-i\varphi}\frac{i\sin\theta}{\sqrt{2}} \end{cases}$

T上升并回落: $\beta(\varepsilon + T + \varepsilon) = -ie^{-i\frac{\delta T}{2}}e^{-i\delta\varepsilon}e^{-i\varphi}\cos\frac{\delta T}{2}$ 即$|\beta(\varepsilon + T + \varepsilon)|^2 = \frac{1 + \cos\delta T}{2}$

L,S,I的耦合: $J = L + S, F = I + J = (L + S) + I$

对$^{87}Rb, I = S_n = \frac{3}{2}, J = S_e = \frac{1}{2}$

$\alpha_{hf} I \cdot J = \alpha_{nf}\frac{(I+J)^2 - I^2 - J^2}{2} = \frac{\alpha_{nf}}{2}(F^2 - I^2 - J^2) = \frac{\alpha_{nf}}{2}[F(F+1) - I(I+1) - J(J+1)]$

$$\alpha^2=\begin{cases}\text{hyperfine} & 10^8\sim 10^9 Hz\\ \text{soc} & 10^{10}\sim 10^{11} Hz(meV)\\ \text{Coulomb} & 10^{14} Hz(eV)\end{cases}$$

$H_{Zeeman}=B(\mu_B g_s S_z+\mu_N g_I I_z),\quad B\to\infty, H_N^2\ll H_e^2$

SI: $\mu_B=\frac{e\hbar}{2m},\mu_N=\frac{e\hbar}{2m_p}$ CGS: $\mu_B=\frac{e\hbar}{2mc},\mu_N=\frac{e\hbar}{2m_pc}$

$H_{Zeeman}(B\to\infty)\sim B\mu_B g_s S_z$

$\boldsymbol{\nabla}\cdot\vec{B}=0,\boldsymbol{\nabla}\times\vec{B}=0\implies\nabla^2\vec{B}=0\quad|B|$没有极大值，HFS(超精细态)不能被磁阱束缚

$|\vec{B}|=\sqrt{B_x^2+B_y^2+B_z^2}$,而

$$\begin{aligned}\partial_x^2|\vec{B}|&=-\frac{1}{|\vec{B}|^3}(B_i\partial_x B_i)^2+\frac{1}{|\vec{B}|}[\sum_i(\partial_x B_i)^2+B_i\partial_x^2 B_i]\\&\geq-\frac{1}{|\vec{B}|^3}(B_iB_i)[\sum_i(\partial_x B_i)^2]+\frac{1}{|\vec{B}|}[\sum_i(\partial_x B_i)^2+B_i\partial_x^2 B_i]\\&=-\frac{1}{|\vec{B}|}B_i\partial_x^2 B_i\end{aligned}$$

即$\nabla^2|\vec{B}|\geq-\frac{1}{|\vec{B}|}(B_i\nabla^2 B_i)=0$，故$|\vec{B}|$只有极小值

$\nabla^2\vec{B}=0\implies\nabla^2 B_x=\nabla^2 B_y=\nabla^2 B_z=0$

例如$B=B_0(x,y,-2z)\,H(\vec{r})=\alpha_{hf}I\cdot J+\vec{B}(\vec{r})\cdot(\mu_B g_s\vec{S}+\mu_N g_N\vec{I})$

对角化$U^\dagger(r)H(r)U(r)=\mathrm{diag}\{\Lambda_1\cdots\Lambda_q\}|B(\vec{r})|$

令$H'=U^\dagger HU,\tilde{\psi}=U^\dagger\psi$ 有$i\hbar\frac{\partial}{\partial t}\tilde{\psi}=H'\tilde{\psi}$

及$U^\dagger pU=\vec{p}-\vec{A},\quad\vec{A}=i\hbar U^\dagger(r)\nabla U(\vec{r})$ 即$\frac{1}{2m}p^2\to\frac{1}{2m}(\vec{p}-\vec{A})^2$

最后得到 $i\hbar\frac{\partial\tilde{\psi}}{\partial t}=[\frac{1}{2m}(-i\hbar\nabla-\vec{A})^2+\Lambda(r)]\tilde{\psi}$，其中$\Lambda(r)=U^\dagger(\vec{r})H_s(\vec{r})U(\vec{r})$

对偶核 $ap+bn\leftrightarrow an+bp\ V_{p-p}\approx V_{p-n}\approx V_{n-n}$

isospin $I=\frac{1}{2}\quad\binom{p}{n}\quad p:I_s=\frac{1}{2},\uparrow\quad n:I_s=-\frac{1}{2},\downarrow$

双原子和多原子分子　电子-转动:spin-rot 电子-振动：SSB,Higgs 振动-转动：Coriolis

$H_N=-\frac{\hbar^2}{2m_a}\nabla_a^2-\frac{\hbar^2}{2m_b}\nabla_b^2+U(R)$

$H=H^{rot}+H^{vib},\quad H^{rot}=\frac{1}{2}\Omega^T I\Omega=\frac{L^2}{2\mu R^2}$

$H^{vib}=-\frac{\hbar^2}{2\mu}\nabla^2+U(R),\quad\psi(R,\theta,\varphi)=F(R)Y_J^\mu(\theta,\varphi)$

$G(R)=RF(R),\quad-\frac{\hbar^2}{2\mu}G''+\left[\frac{J(J+1)\hbar^2}{2\mu R^2}+U(R)-E\right]G(R)=0$

令$R-R_e=q,\quad U(R)=U_0+\frac{1}{2}kq^2$ 记$S(q)=G(R)$则

$-\frac{\hbar^2}{2\mu}S''(q)+\frac{1}{2}(kq^2-W)S(q)=0,\quad W=E-U(R_e)-\frac{J(J+1)\hbar^2}{2\mu R_e^2}$

得$S_\nu(q)=\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^\nu\nu!}}H_\nu(\sqrt{\alpha}q)e^{-\frac{1}{2}\alpha q^2},\quad\alpha=\frac{4\pi\nu_e\mu}{h},\nu_e=\frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$

考虑转动部分$H=-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}q^2}+\frac{1}{2}kq^2+\frac{J^2}{2\mu R_e^2}-q\frac{J^2}{\mu R_e^3}$

即$H=-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}q^2}+\frac{1}{2}k(q-\frac{J^2}{\mu k R_e^2})^2-\frac{J^4}{2\mu^2 k R_e^6}+\frac{J^2}{2\mu R_e^2}$

Huang-Rhys电声耦合理论　Franck-Condon: $|\langle\nu'|H|\nu\rangle|^2\propto|\langle\nu'|\nu\rangle|$

$\mu=\mu_e+\mu_N$,而

$$\begin{aligned}\langle\mu\rangle&=\int\psi_{el}'^*\psi_{\nu'}'(\mu_e+\mu_N)\psi_{el}\psi_\nu\mathrm{d}r\mathrm{d}R\\&=\int\psi_{\nu'}'^*\psi_\nu\mathrm{d}R\int\psi_{el}'^*\mu_e\psi_{el}\mathrm{d}r+\int\psi_{el}'^*\psi_{el}\mathrm{d}r\int\psi_{\nu'}'\mu_N\psi_\nu\mathrm{d}R\\&=_e\langle\nu'|\nu\rangle_q\int\psi_{el}'^*\mu_e\psi_{el}\mathrm{d}r\end{aligned}$$

总哈密顿量

$$H=-\frac{\hbar^2}{2m}\sum_i^{el}\nabla_i^2-\frac{\hbar^2}{2}\sum_\alpha^{Nucl}\frac{1}{m_\alpha}\nabla_\alpha+\sum_\alpha\sum_{p>\alpha}\frac{Z_\alpha Z_\beta e^2}{R_{\alpha\beta}}-\sum_\alpha\sum_i\frac{Z_\alpha e^2}{r_{i\alpha}}+\sum_i\sum_{j>i}\frac{e^2}{r_{ij}}$$

$H(r_i,R_\alpha)\psi(r_i,R_\alpha)=E(r_i,R_\alpha)$

Born-Oppenheimer Ansatz(预解式)　$\psi(r_i,R_\alpha)=\sum_I\psi_{el,I}(r_i,R_\alpha)\psi_{N,I}(R_\alpha)$

$H_{el}\psi_{el,I}=E_O(R_\alpha)\psi_{el,I},\quad U_I=E_{el,I}+V_{NN}$，$E_{el,I}$为1,4,5部分，$V_{NN}$为3部分

$H_N=-\frac{\hbar^2}{2}\sum_\alpha\frac{1}{m_\alpha}\nabla_\alpha^2+U_I(R_\alpha)$

$I=0$:

$$\begin{aligned}-i\frac{\partial}{\partial t}\psi_{N,0}=&-\frac{\hbar^2}{2m_\alpha}\left(\frac{\partial^2}{\partial R_\alpha^2}\psi_{N,0}+2\frac{\partial\psi_{N,0}}{\partial R_\alpha}\sum_I\langle\psi_{el,0}|\frac{\partial}{\partial R_\alpha}|\psi_{el,0}\rangle+\langle\psi_{el,0}|\frac{\partial^2}{\partial R_l^2}|\psi_{el,0}\rangle\psi_{N,0}\right)\\&+U_0(R_\alpha)\psi_{N,0}\end{aligned}$$

其中$\langle\psi_{el,0}|\frac{\partial^2}{\partial R_l^2}|\psi_{el,0}\rangle$称为Born-Huang connection

$R_0\to R_0'$ $(\hat{D})$: 电声耦合激发 $\omega\to\omega'(\hat{S})$: 压缩态　$\{S_i\}\to\{S_i'\}(\hat{U})$: 模式切换

$\xi=1,\cdots,f$ $C_\xi^{(r)}=\sqrt{\frac{\omega}{2\hbar}}q_\xi+i\frac{1}{\sqrt{2\hbar\omega}}p_\xi$　即$\begin{cases}q_\xi=\sqrt{\frac{\hbar}{2\omega}}(c_\xi+c_\xi^\dagger)\\p_\xi=-i\sqrt{\frac{\hbar\omega}{2}}(c_\xi-c_\xi^\dagger)\end{cases}$

引入$\begin{cases}Q_\xi=q_\xi\sqrt{\frac{2\omega}{\hbar}}=c_\xi+c_\xi^\dagger\\P_\xi=p_\xi\sqrt{\frac{2}{\hbar\omega}}=-i(c_\xi-c_\xi^\dagger)\end{cases}$

本征态$|v_1\cdots v_f\rangle$，对双原子分子记为$|\nu_1\rangle$　$c_\xi|v_\xi\rangle=\sqrt{v_\xi}|v_\xi-1\rangle,c_\xi^\dagger|v_\xi\rangle=\sqrt{v_\xi+1}|v_\xi+1\rangle$

$H_{e/g}=U(q_{\xi,0}^{(e/g)})+\frac{1}{2}\sum_\zeta(p_\zeta^2+\omega_\zeta^2(q_\zeta-q_{0,\zeta}^{(e/g)})^2)$

定义$g_a^{(\zeta)}=-\sqrt{\frac{\omega}{2\hbar}}q_{\zeta,0}^{(a)},\quad a=e,g$则

$H_a=U_a^{(0)}+\sum_\zeta\hbar\omega_\zeta(c_\zeta^\dagger c_\zeta+\frac{1}{2})+\sum_\zeta\hbar\omega_\zeta(g_a(\zeta)(c_\zeta^\dagger+c_\zeta)+g_a^2(\zeta))$

$|g\rangle,|e\rangle,q=0$　位移为$q_{\zeta,0}^{(a)}$

将含g的项看作微扰，$H=\sum_\zeta \hbar\omega_\zeta(c_\zeta^\dagger c_\zeta+\frac{1}{2})\left|v_\zeta\right\rangle=\frac{1}{\sqrt{v_\zeta!}}(c_\zeta^\dagger)^v\left|0\right\rangle$

相应 $\psi_{a(=e,g),v}(q_\zeta-q_\zeta^{(a)})=\sum_{n=0}^\infty\frac{(-q_\zeta^{(a)})^n}{n!}\frac{\mathrm{d}^n}{\mathrm{d}q_\zeta^n}\psi_{a,v}(q_\zeta)=e^{-\frac{i}{\hbar}q_\zeta^{(a)}\hat{p}_\zeta}\psi_{a,v}(q_\zeta)$

由$-\frac{i}{\hbar}q_\zeta^{(a)}\hat{p}_\zeta=g_a(\zeta)(c_\zeta-c_\zeta^\dagger)$，可知平移算符

$D^\dagger(g_a(\zeta))=e^{g_a(\zeta)(c_\zeta-c_\zeta^\dagger)}$，且$D(g_a(\zeta))\left|0\right\rangle=\left|g_a(\zeta)\right\rangle$

即$\left|v_\zeta^{(a)}\right\rangle=\frac{1}{\sqrt{v_\zeta!}}D^\dagger(g_a(\zeta))(\hat{c}_\zeta^\dagger)^{v_\zeta}\left|0\right\rangle=D^\dagger(g_a(\zeta))\left|v_\zeta\right\rangle$

平移算符满足 $D^\dagger(g)=D(-g)=D^{-1}(g)$

对$c,c^\dagger$的位移 $D^\dagger(g)c^\dagger D(g)=e^{g(c-c^\dagger)}c^\dagger e^{-g(c-c^\dagger)}$

利用BCH公式 $e^ABe^{-A}=B+[A,B]+\frac{1}{2!}[A,[A,B]]+\frac{1}{3!}[A,[A,[A,B]]]+\cdots$

可得 $D^\dagger(g)c^\dagger D(g)=c^\dagger+g$，即$H_a=U_a^{(0)}+\sum_\zeta\hbar\omega_\zeta[(c_\zeta^\dagger+g_a(\zeta))(c_\zeta+g_a(\zeta))+\frac{1}{2}]$

投影 $\left\langle\psi_{e\mu}|\psi_{g\nu}\right\rangle=\left\langle\mu\right|D(g_e)D^\dagger(g_g)\left|\nu\right\rangle$，其中

$D(g_e)D^\dagger(g_g)=e^{-g_e(c-c^\dagger)}e^{g_g(c-c^\dagger)}=e^{\Delta g_{eg}c^\dagger}e^{-\Delta g_{eg}c}e^{-\frac{\Delta g_{eg}^2}{2}}$

其中 $\Delta g_{eg}=g_e-g_g=-\sqrt{\frac{\omega}{2\hbar}}(q_o^{(e)}-q_o^{(g)})$

而 $e^{-\Delta g_{eg}c}\left|\nu\right\rangle=\sum_{n=0}^\nu\frac{(-\Delta g_{eg})^n}{n!}c^n\left|\nu\right\rangle=\sum_{n=0}^\nu\frac{(-\Delta g_{eg})^n}{n!}\sqrt{\frac{\nu!}{(\nu-n)!}}\left|\nu-n\right\rangle$

由此得到

$$\left\langle\psi_{e\nu'}|\psi_{g\nu}\right\rangle=e^{-\frac{\Delta g_{eg}^2}{2}}\sum_{m=0}^{\nu'}\sum_{n=0}^{\nu}\frac{(-)^n(\Delta g_{eg})^{m+n}}{m!n!}\sqrt{\frac{\nu'!}{(m-\nu')!}\frac{\nu!}{(n-\nu)!}}\delta_{\nu'-m,\nu-n}$$

对$\nu=0\implies n=0$，定义$\Delta g_{eg}^2=\frac{\omega}{2\hbar}(\Delta q_o^2)=S$

则 $|\left\langle\psi_{e\nu'}|\psi_{g0}\right\rangle|^2=e^{-S}\left(\sum_{m=0}\frac{(\sqrt{S})^m}{m!}\sqrt{\frac{\nu'!}{(m-\nu')!}}\delta_{\nu'-m,0}\right)^2=\frac{e^{-S}S^{\nu'}}{\nu'!}$即$|\left\langle\nu|0\right\rangle|^2=\frac{e^{-S}S^\nu}{\nu!}$，$S\ll 1$时，对$\nu\neq 0$将压低投影概率

$\hat{D}^\dagger(g)\hat{q}\hat{D}(g)=\hat{q}+g$平移 $\hat{S}^\dagger(\lambda)\hat{q}\hat{S}(\lambda)=e^\Lambda\hat{q}$压缩（拉伸） $\hat{U}^\dagger(0)\hat{q}\hat{U}(0)=\hat{O}\hat{q}$

$\hat{q}_{e,0}=Aq_{g,0}+d=\hat{W}^\dagger q_{g,0}\hat{W},\quad \hat{W}\approx\hat{U}(0)\hat{S}(\lambda)\hat{D}(g)$

由$\left\langle\nu_e'|\nu_g\right\rangle=\left\langle 0_e\right|\prod_{s=1}^f\frac{c_{e,\zeta}^{\nu_\zeta}}{\sqrt{\nu_\zeta!}}\left|\nu_g\right\rangle$，可知

$$\begin{aligned}\left\langle\nu_1'\nu_2'\cdots|\nu_1\nu_2\cdots\right\rangle&=\left\langle 0_g\right|\hat{W}\left(\hat{W}^T\prod_{\zeta=1}^f\frac{c_{g,\zeta}^{\nu_\zeta}}{\sqrt{\nu_\zeta!}}\hat{W}\right)\left|\nu_g\right\rangle\\&=\left\langle 0_g\right|\prod_{\zeta=1}^f\frac{c_{g,\zeta}^{\nu_\zeta}}{\sqrt{\nu_\zeta!}}\hat{W}\left|\nu_g\right\rangle\\&=\left\langle\nu_g'\right|\hat{W}\left|\nu_g\right\rangle\end{aligned}$$

考虑电磁波，$(x,p)\leftrightarrow(E,\varphi),\quad\tilde{E}=Ee^{i\varphi}$

$\hat{\vec{E}}(\vec{r},t)=\hat{\vec{E}}^{(+)}(\vec{r},t)+\hat{\vec{E}}^{(-)}(\vec{r},t),\quad(E^{(-)})=(E^{(+)})^\dagger$

$E^{(+)}$: photon absorption, $n\to n-1$ $\quad E^{(-)}$: photon emission, $n\to n+1$

即$E^{(+)}\sim\hat{a}e^{-i\omega t}$, $E^{(-)}\sim\hat{a}^\dagger e^{i\omega t}$, $\hat{\vec{E}}^{(+)}\left|vac\right\rangle=0$, $\left\langle vac\right|\hat{\vec{E}}^{(-)}=0$

一阶关联函数 $\quad G^{(1)}_{\mu\nu}(\vec{r}t,\vec{r}'t')=\mathrm{Tr}[\hat{\rho}\hat{E}^{(-)}_\mu\hat{E}^{(+)}_\nu]=\mathcal{E}^*_\mu(\vec{r}t)\mathcal{E}_\nu(\vec{r}'t')$

给定$(\omega,\vec{k},\hat{e}^{(\lambda)},\vec{\mathcal{E}})$，单模自由空间电磁波满足

$$\nabla^2\vec{u}_k+\frac{\omega_k^2}{c^2}\vec{u}_k=0,\begin{cases}\nabla\cdot\vec{u}_k=0\\ \int\vec{u}^*_k(\vec{r})\vec{u}_l(\vec{r})\,\mathrm{d}\vec{r}=\delta_{kl}\end{cases}$$

得$\vec{u}_k(\vec{r})=\frac{1}{L^{\frac{3}{2}}}\hat{e}^{(\lambda)}e^{i\vec{k}\cdot\vec{r}}$, $\lambda=1,2$为偏振自由度

对应 $\hat{\vec{A}}=c\sum_k\sqrt{\frac{\hbar}{2\omega_k}}[\hat{a}_k\vec{u}_k(\vec{r})e^{-i\omega_k t}+\hat{a}^\dagger_k\vec{u}_k(\vec{r})e^{i\omega_k t}]$

因此 $\hat{H}=\frac{1}{2}\int(E^2+B^2)\,\mathrm{d}\vec{r}=\frac{1}{2}\sum_k\hbar\omega_k(a^\dagger_ka_k+a_ka^\dagger_k)=\sum_k\hbar\omega_k(n_k+\frac{1}{2})$

对易关系 $[\hat{a}_k,\hat{a}^\dagger_{k'}]=\delta_{k'k},\quad[\hat{a}_k,\hat{a}_{k'}]=[\hat{a}^\dagger_k,\hat{a}^\dagger_{k'}]=0$

本征态 $\hat{a}_k|0\rangle_k=0,\quad|n_k\rangle_k=\frac{(\hat{a}^\dagger_k)^{n_k}}{(n_k!)^2}|0\rangle_k,\quad\begin{cases}\hat{a}_k|n_k\rangle_k=\sqrt{n_k}|n_k-1\rangle_k\\ \hat{a}^\dagger_k|n_k\rangle_k=\sqrt{n_k+1}|n_k+1\rangle_k\\ \hat{a}^\dagger_k\hat{a}_k|n_k\rangle_k=n_k\,|n_k\rangle\end{cases}$

电场$\hat{\vec{E}}=-\frac{1}{c}\frac{\mathrm{d}\hat{\vec{A}}}{\mathrm{d}t},\quad\hat{\vec{E}}^{(+)}(\vec{r}t)=i\sum_k\sqrt{\frac{\hbar\omega_k}{2}}\hat{a}_k\vec{u}_k(\vec{r})e^{-i\omega_k t}$

电场算符的本征态：考虑相干态$\hat{a}\left|\alpha\right\rangle=\vec{\alpha}\left|\alpha\right\rangle$

$\sqrt{n+1}\langle n+1\left|\alpha\right\rangle=\alpha\left\langle n|\alpha\right\rangle\implies\left\langle n|\alpha\right\rangle=\frac{\alpha^n}{\sqrt{n!}}\langle0|\alpha\rangle$

$\left|\alpha\right\rangle=\sum_n|n\rangle\langle n|\alpha\rangle=\langle0\left|\alpha\right\rangle\sum_n\frac{\alpha^n}{\sqrt{n!}}|n\rangle$

而$\langle\alpha\left|\alpha\right\rangle=|\left\langle0|\alpha\right\rangle|^2\sum_n\frac{|\alpha|^{2n}}{n!}=|\left\langle0|\alpha\right\rangle|^2e^{|\alpha|^2}$

归一化：$\langle\alpha|\alpha\rangle=1\implies\langle0|\alpha\rangle=e^{-\frac{|\alpha|^2}{2}}\implies|\alpha\rangle=e^{-\frac{|\alpha|^2}{2}}\sum_n\frac{\alpha^n}{\sqrt{n!}}|n\rangle$

由$q=\sqrt{\frac{\hbar}{2\omega}}(\hat{a}^\dagger+\hat{a}),p=i\sqrt{\frac{\hbar\omega}{2}}(\hat{a}^\dagger-\hat{a}),[q,p]=i\hbar$

可得 $\langle\alpha|q\left|\alpha\right\rangle=\sqrt{\frac{2\hbar}{\omega}}\mathrm{Re}\alpha,\quad\langle\alpha|p\left|\alpha\right\rangle=\sqrt{2\hbar\omega}\mathrm{Im}\alpha$

考虑$\hat{a}\vec{u}_k(\vec{r})=\alpha\vec{u}_k(\vec{r})=\mathcal{E}_\alpha u_k(\vec{r})$，含相互作用的哈密顿量

$\hat{H}=\hat{H}_{rad}+\hat{V}(t)=\hbar\omega(\hat{a}^\dagger\hat{a}+\frac{1}{2})+i\hbar(f(t)\hat{a}^\dagger-f^*(t)\hat{a}),\quad f(t)=f_0e^{-i\omega t}$

相互作用表象中 $V_I(t)=e^{\frac{iH_0t}{\hbar}}i\hbar(f(t)\hat{a}^\dagger-f^*(t)\hat{a})e^{-\frac{iH_0t}{\hbar}}=i\hbar(f_0\hat{a}^\dagger-f_0^*\hat{a})$

演化算符 $i\hbar\frac{\partial}{\partial t}U_I=V_IU_I\implies U_I(t)=e^{(f_0\hat{a}^\dagger-f_0^*\hat{a})t}$

相应 $\left|\psi(t)\right\rangle_I=e^{(f_0t)\hat{a}^\dagger-(f_0^*t)\hat{a}}\left|0\right\rangle=D(f_0t)\left|0\right\rangle=e^{-\frac{|f_0|^2t^2}{2}}e^{f_0a^\dagger t}\left|0\right\rangle$ 是相干态

$D(\alpha)=e^{\alpha\hat{a}^\dagger-\alpha^*\hat{a}},\quad\left|\alpha\right\rangle=D(\alpha)\left|0\right\rangle$

单位分解：$1=\sum_n\left|n\right\rangle\left\langle n\right|=\frac{1}{\pi}\int\mathrm{d}^2\alpha\left|\alpha\right\rangle\!\left\langle\alpha\right|$

相干态展开 $\left|\psi\right\rangle=\int\mathrm{d}^2\alpha F(\alpha)\left|\alpha\right\rangle$

压缩相干态 $H=\frac{p^2}{2}+\frac{1}{2}\omega^2q^2=\frac{p^2}{2}+\frac{1}{2}Cq^2,\quad H'=\frac{p^2}{2}+\frac{1}{2}\omega'^2q^2=\frac{p^2}{2}+\frac{1}{2}C'q^2$

$H' = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) + \frac{1}{2}C_1 q^2 = \hbar\tilde{\omega}(\hat{a}^\dagger\hat{a} + \frac{1}{2}) + \frac{1}{2}\tilde{C}_1(\hat{a}^{\dagger 2} + \hat{a}^2)$

压缩算符 $\hat{S}(\zeta) = e^{\frac{\zeta\hat{a}^{\dagger 2} - \zeta^*\hat{a}^2}{2}}, \zeta = re^{i\varphi}$

$\hat{Q} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger), \hat{P} = \frac{1}{\sqrt{2}i}(\hat{a} - \hat{a}^\dagger),$

对压缩态 $\hat{Q}(r) = \hat{S}^\dagger(r)\hat{Q}(0)\hat{S}(r) = Q(0)e^{-r}, \quad \hat{P}(r) = \hat{S}^\dagger(r)\hat{P}(0)\hat{S}(r) = P(0)e^r$

升降算符 $\hat{a}(r) = \hat{a}\cosh r - \hat{a}^\dagger\sinh r, \quad \hat{a}^\dagger(r) = -\hat{a}\sinh r + \hat{a}^\dagger\cosh r$

考虑频率突变的振子 $H(t) = \hbar\omega(t)(\hat{a}^\dagger\hat{a} + \dfrac{1}{2}), \quad \omega(t) = \begin{cases} \omega_0, & t < 0 \\ \omega_1, & t \geq 0 \end{cases}$

升降算符 $\begin{cases} \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega_0}{\hbar}}\hat{Q} - i\sqrt{\frac{1}{\hbar m\omega_0}}\hat{P}) \\ \hat{a} = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega_0}{\hbar}}\hat{Q} + i\sqrt{\frac{1}{\hbar m\omega_0}}\hat{P}) \end{cases}$

演化

$$\begin{aligned}
\hat{\tilde{a}}^\dagger(t) &= e^{i\omega_1 t}\hat{a}^\dagger(0) \\
&= e^{i\omega_1 t}\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_1}{\hbar}}\hat{Q} - i\sqrt{\frac{1}{m\hbar\omega_1}}\hat{P}\right) \\
&= e^{i\omega_1 t}\frac{1}{\sqrt{2}}\left[\sqrt{\frac{\omega_1}{\omega_0}}\sqrt{\frac{m\omega_0}{\hbar}}\hat{Q} - i\sqrt{\frac{\omega_0}{\omega_1}}\sqrt{\frac{1}{m\hbar\omega_0}}\hat{P}\right] \\
&= e^{i\omega_1 t}\left(\frac{\omega_1 + \omega_0}{2\sqrt{\omega_0\omega_1}}\hat{a}^\dagger + \frac{\omega_1 - \omega_0}{2\sqrt{\omega_0\omega_1}}\hat{a}\right) \\
&= U^*(t)\hat{a}^\dagger + V^*(t)\hat{a}
\end{aligned}$$

写成压缩参数形式

$$\begin{cases} \hat{\tilde{a}}^\dagger(0) = \cosh r\hat{a}^\dagger - \sinh r\hat{a} \\ \hat{\tilde{a}}(0) = \cosh r\hat{a} + \sinh r\hat{a}^\dagger \end{cases}$$

其中压缩参数$r = \operatorname{arctanh}\frac{\omega_0 - \omega_1}{\omega_0 + \omega_1}$, $S = -10\lg e^{-2r}(dB)$

以及 $\langle Q^2\rangle(t) = \frac{\hbar}{2m\omega_1}\langle(\tilde{a}(t) + \tilde{a}^\dagger(t))^2\rangle = \frac{\hbar}{m\omega_1}\langle|U(t) + V^*(t)|^2(n + \frac{1}{2})\rangle,$

其中 $\langle n + \frac{1}{2}\rangle = \frac{1}{e^{\beta\hbar\omega_0 - 1}} + \frac{1}{2} = \frac{1}{2}\coth\frac{\beta\hbar\omega_0}{2},$

以及 $|U(t) + V^*(t)|^2 = \frac{\omega_1}{2\omega_0}\left[\left(1 + \frac{\omega_0^2}{\omega_1^2}\right) + \left(1 - \frac{\omega_0^2}{\omega_1^2}\right)\cos 2\omega_1 t\right]$

Fiber bundle & vibration

考虑甲烷分子，$M = \{c, H_1, H_2, H_3, H_4\}$，对应$E_c, E_1, E_2, E_3, E_4$

给定位移函数f即平衡位置附近的位移，$f(c) \in E_c, f(i) \in E_i, i = 1, 2, 3, 4$

抽象化：

$M = \{x\}$, 定义vector bundle, 矢量空间的集合 $\{E_x\}, \forall x \in M$

$E = \bigcup_{x \in M} E_x$ 是M上的VBun，不是矢量空间

$\pi : E \to M, \pi(v) = x, v \in E_x \quad E_x = \pi^{-1}(x)$是$x$点的纤维

(E,M) VBun 截面f是M上的函数，$f(x)\in E_x,\forall x\in E_x$

$(f_1+f_2)(x)=f_1(x)+f_2(x),\quad (cf)(x)=c(f(x)),\Gamma=\{f_i\}$

$\dim(\Gamma(E))=\sum_{x\in M}\dim(E_x)$

G作用于M，E是M上Bun_V，G作用如下：

(1)$a\in G,E_x\to E_{ax}$是线性的；(2)$\pi:E\to M$是$G-$态射，$a\pi(v)=\pi(av)$

$\Gamma(E)$是$3N$维线性空间，可作为G的表示空间

对于不变原子$ax=x,a(v_x)_j=\sum_i(A_x)_{ij}(v_x)_i\implies af_{v_{xj}}=\sum_i(A_x)_{ij}f_{v_{xi}}$

$R(a)$在$\Gamma(E)$截面上作用的特征标$\chi=\sum_{x,i}(A_x)_{ii}$

$Frob_a(M)=\{x\in M|ax=x\}$

Frobenius不动点定理：对$a\in G,\chi_E(a)$特征标为 $\chi_E(a)=\sum_{x\in Frob_a(M)}\mathrm{Tr}(a:E_x\to E_x)$

特征标表：

T_a	E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
$R_xR_yR_z(T_1)$	3	0	-1	-1	1
$xyz(T_2)$	3	0	-1	-1	1
Γ	3	0	-1	1	-1

$\chi(C_n^m)=N_{C_n^m}^{inv}[1+2\cos\frac{2n\pi}{m}],\chi(E)=3N,\chi(S_n)=\chi(C_n\sigma_n)=N_{S_n}^{inv}(-1+2\cos\frac{2\pi}{n})$

$\chi(i)=-3N_i^{inv},\chi(\sigma)=N_\sigma^{inv},\chi(\sigma_d)=N_{\sigma_d}^{inv}$

$\Gamma=A_1\oplus E\oplus T_1\oplus 3T_2,\quad \Gamma_{vib}=T-T_1-T_2=A_1\oplus E\oplus 2T_2$

分子的转动

双原子 $\vec{J}=\vec{N}+\vec{L}+\vec{S}$, $\vec{N}$为机械部分

$\hat{H}=B\hat{N}^2=B(N_x^2+N_y^2)=B(\vec{J}-\vec{L}-\vec{S})_{x,y}^2$

$$\begin{aligned}\hat{H}_{rot}&=B(J^2-J_z^2)+B(S^2-S_z^2)+B(L^2-L_z^2)\\&-B(J^+L^-+J^-L^+)-B(J^+S^-+J^-S^+)+B(L^+S^-+L^-S^+)\end{aligned}$$

$\hat{H}_{SO}=A\vec{L}\cdot\vec{S}=AL_zS_z+\frac{1}{2}A(L^+S^-+L^-S^+)$

角动量升降 $J^{\mp}\left|\Omega JM\right\rangle=\hbar\sqrt{J(J+1)-\Omega(\Omega\pm1)}\left|\Omega\pm1,JM\right\rangle$

Anomalous commutator $[\hat{J}_x,\hat{J}_y]=-i\hbar\hat{J}_z$

$\hat{e}_i,i=X,Y,Z\ \ \hat{u}^\alpha,\alpha=x,y,z$ 方向余弦 $\lambda_{\alpha i}=\hat{u}^\alpha\cdot\hat{e}_i$

$[J_\alpha,J_\beta]=-i\hbar\varepsilon_{\alpha\beta\gamma}K_\gamma,\quad [J_x,J_y]=[\lambda_{xi}J_i,\lambda_{yj}J_j]$

利用$\lambda_{xY}\lambda_{yZ}-\lambda_{xZ}\lambda_{yY}=\lambda_{zZ}$可得 $[\hat{J}_x,\hat{J}_y]=-i\hbar\hat{J}_z$

考虑$^2\Sigma^+$: $\left|^2\Sigma_{\pm\frac{1}{2}}\right\rangle=\left|\Lambda=0,S=\frac{1}{2},\Sigma=\pm\frac{1}{2}\right\rangle\left|\Omega=\pm\frac{1}{2},JM\right\rangle$

$\left\langle ^2\Sigma_{\frac{1}{2}}\middle|\hat{H}_{rot}\middle|^2\Sigma_{\frac{1}{2}}\right\rangle=\left\langle ^2\Sigma_{-\frac{1}{2}}\middle|\hat{H}_{rot}\middle|^2\Sigma_{-\frac{1}{2}}\right\rangle=B(J+\frac{1}{2})^2$

$\left\langle ^2\Sigma_{-\frac{1}{2}}\middle|\hat{H}_{rot}\middle|^2\Sigma_{\frac{1}{2}}\right\rangle=-B(J+\frac{1}{2})$

即 $H=\begin{pmatrix}B(J+\frac{1}{2})^2 & -B(J+\frac{1}{2})\\ -B(J+\frac{1}{2}) & B(J+\frac{1}{2})^2\end{pmatrix}$

新基 $\left|^2\Sigma^+(e,f)\right\rangle=\frac{\left|^2\Sigma^+_{\frac{1}{2}}\right\rangle\pm\left|^2\Sigma^+_{-\frac{1}{2}}\right\rangle}{\sqrt{2}}$，在此基下对角化

$H=\begin{pmatrix}B(J+\frac{1}{2})^2-B(J-\frac{1}{2}) & 0\\ 0 & B(J+\frac{1}{2})^2-B(J+\frac{1}{2})\end{pmatrix}$

$\vec{N}=\vec{J}-\vec{S},\ N=J-\frac{1}{2},|e\rangle;N=J+\frac{1}{2},|f\rangle$

$F_1(e)=BN(N+1)=F_2(f)$

加入电场，$\mu\cdot E=\mu_zE_z$

$\mu_Z^{lab}=\mu_i\cos iZ=(\alpha_{zz}E_z)_{lab}=\alpha_{ii}E_i\cos(iZ)=\alpha_{ii}E_Z\cos^2(iZ)=E_z(\alpha_{xx}+(\alpha_{yy}-\alpha_{xx})\cos^2(zZ))$

考虑水分子，$\hat{H}=\hat{H}_{rot}+\hat{H}'=\hat{H}_{rot}-E_i^*(t)\alpha_{ij}E_j(t),\alpha_{ij}$为实验室系中

即$\hat{H}'=-\frac{1}{2}\sum_{JM}(-)^{J+M}U(t)_M^{[J]}\alpha_{-M}^{[J]},U(t)_M^{[J]}=[E^*(t)^{[1]}\times E(t)^{[1]}]_M^{[J]}$

其中$T_q^{[1]}=\begin{cases}-\frac{T_x+iT_y}{\sqrt{2}} & q=1\\ T_z & q=0\\ \frac{T_x-iT_y}{\sqrt{2}} & q=-1\end{cases}$

张量积 $\{E^{[1]}\times E^{[1]}\}_M^{[J]}=\sum_{q_1q_2}\langle 1q_11q_2|11JM\rangle E_{q_1}^{[1]}E_{q_2}^{[1]}$

$(E^{[1]}\times E^{[1]})_0^0=\sum_{q_1q_2}\begin{pmatrix}1&1&0\\q_1&q_2&0\end{pmatrix}E_{q_1}^{[1]}E_{q_2}^{[1]},\quad \begin{pmatrix}1&1&0\\q_1&q_2&0\end{pmatrix}=(-)^{1-q_1}\delta_{q_1-q_2}\frac{1}{\sqrt{3}}$

$E(t)=(\pm E_x\sin(k_yy-\omega t),0,E_z\cos(k_yy-\omega t))=\frac{1}{2}(\pm E_x,0,E_z)$

$(E^{[1]}\times E^{[1]})_0^0=-\frac{1}{\sqrt{3}}(E_x^2(t)+E_z^2(t))$

$|E(t)|^2=E_x^2\sin^2(k_yy-\omega t)+E_z\cos^2(k_yy-\omega t)=4\pi\alpha I$

$a=\frac{E_x}{\sqrt{E_x^2+E_z^2}},b=\frac{E_z}{\sqrt{E_x^2+E_z^2}},E=\sqrt{4\pi\alpha I}(\pm a,0,b)$

$U_0^{[0]}=-\frac{1}{\sqrt{3}}(E_x^2(t)+E_z^2(t))=-\sqrt{\frac{1}{3}}4\pi\alpha I,U_0^{[2]}(t)=\sqrt{\frac{1}{6}}(2E_z^2(t)-E_x^2(t))=\sqrt{\frac{1}{6}}4\pi\alpha I(2-3a^2)$

$U_{\pm1}^{[2]}=\mp E_x(t)E_z(t)=0\ U_{\pm2}^{[2]}=\frac{1}{2}E_x^2(t)=2\pi\alpha Ia^2$ (时间平均)

$\alpha^{(p)}=\begin{pmatrix}\alpha_R&&\\&\alpha_S&\\&&\alpha_T\end{pmatrix}$

$\alpha_0^{(0)}=-\sqrt{\frac{1}{3}}(\alpha_R+\alpha_S+\alpha_T)\quad \alpha_0^{(2)}=\sqrt{\frac{1}{6}}(2\alpha_T-\alpha_R-\alpha_S)$

$\alpha_{\pm 2}^{(2)}=\frac{1}{2}(\alpha_R-\alpha_S\pm i(\alpha_{RS}+\alpha_{SR}))\quad \alpha_0^{(1)}=\frac{i}{\sqrt{2}}(\alpha_{RS}-\alpha_{SR})$

$\alpha_{\pm 1}^{(1)}=\frac{1}{2}(\alpha_{TR}-\alpha_{RT}\mp i(\alpha_{ST}-\alpha_{TS}))$

$\alpha_{\pm 1}^{(2)}=\mp\frac{1}{2}(\alpha_{RT}+\alpha_{TR}-i(\alpha_{ST}+\alpha_{TS}))$

$\alpha_0^{(0)L}=D_{00}^{(0)}(R_{PL}\alpha_{(0)}^{(0)P})=\alpha_0^{(0)P}$

$\alpha_0^{(2)L}=D_{Q0}^{(2)}(R_{PL})\alpha_Q^{(2)P}=(D_{20}^{(2)}+D_{-20}^{(2)})(R_{PL})\alpha_2^{(2)P}+D_{00}^{(2)}(R_{PL})\alpha_0^{(2)P}$

$\alpha_{\pm 1}^{(2)L}=D_{Q\pm 1}^{(2)}(R_{PL})\alpha_Q^{(2)},\quad \alpha_{\pm 2}^{(2)L}=D_{Q\pm 2}^{(2)}(R_{PL})\alpha_Q^{(2)}$

$H_L=-\frac{1}{2}E_i^{(L)}E_j^{(L)}\alpha_{ij}^{(L)}=-\frac{1}{2}U_{ij}\alpha_{ij}=-\frac{1}{2}\sum_{JM}(-)^{J+M}U_M^{(J)}\alpha_{-M}^{(J)},J=0,2$

即$H_L=-\frac{1}{2}[U_0^{(0)}\alpha_0^{(0)}+U_0^{(0)}\alpha_0^{(0)}+U_2^{(2)}(\alpha_2^{(2)}+\alpha_{-2}^{(2)})]$

考虑转动

$\alpha_0^{(2)L}=D_{m0}^{(2)}(0,\beta,0)\alpha_m^{(2)P}=\sqrt{\frac{4\pi}{3}}Y_{2m}^*(\beta,0)\alpha_m^{(2)P}=\sqrt{\frac{3}{2}}\cos^2\theta(\alpha_{zz}-\alpha_{xx})-\sqrt{\frac{1}{6}}(\alpha_{zz}-\alpha_{xx})$

$\alpha_0^{(2)P}=\sqrt{\frac{1}{6}}(2\alpha_T-\alpha_R-\alpha_S)=\sqrt{\frac{2}{3}}(\alpha_{zz}-\alpha_{xx})$

$\alpha_{\pm 2}^{(2)}=\frac{1}{2}(\alpha_R-\alpha_S\pm i(\alpha_{RS}+\alpha_{SR}))=0$

$\alpha_0^{(0)L}=\alpha_0^{(0)P}=-\sqrt{\frac{1}{3}}(\alpha_{zz}-2\alpha_{xx})$

$U_0^{(2)L}=\sqrt{\frac{1}{6}}(2E_z^2-E_x^2)=\sqrt{\frac{2}{3}}E_z^2,\quad E_x=0$

$U_0^{(0)L}=-\sqrt{\frac{1}{3}}E_z^2$

即$H_L=-\frac{1}{2}\cos^2\theta E_z^2(\alpha_{zz}-\alpha_{xx})+E_z^2\alpha_{xx}$

转动部分 $H=\frac{J_a^2}{2I_{aa}}+\frac{J_b^2}{2I_{bb}}+\frac{J_c^2}{2I_{cc}}=AJ_a^2+BJ_b^2+CJ_c^2,\quad J_a=I_{aa}\omega_a$

设$A\geq B\geq C$即$I_{aa}\leq I_{bb}\leq I_{cc}$

线型：$I_{cc}=I_{bb}>I_{aa}=0$ 球对称分子：$I_{aa}=I_{bb}=I_{cc}$

prolate: $A>B=C,I_{aa}<I_{bb}=I_{cc}$ oblate: $A=B>C,I_{aa}=I_{bb}<I_{cc}$

$\hat{H}^{(pro)}=AJ_a^2+B(J_b^2+J_c^2)=BJ^2+(A-B)J_a^2$

$\hat{H}^{(obl)}=B(J^2-J_c^2)+CJ_c^2=BJ^2+(C-B)J_c^2$

$J^2D_{mk}^{*J}=J(J+1)\hbar^2D_{mk}^{*J},\quad J_zD_{mk}^{*J}=k\hbar D_{mk}^J$

$E^{(pro)}=BJ(J+1)\hbar^2+(A-B)k^2\hbar^2,\quad E^{(obl)}=BJ(J+1)\hbar^2-(B-C)k^2\hbar^2$

$A\neq B\neq C$: 不对称陀螺分子　不对称度$K=\frac{2B-A-C}{A-C}$

长陀螺$A>B=C,K=-1$　扁陀螺$A=B>C,K=1$

$H_{rot}^{obl}=AJ_a^2+BJ_b^2+CJ_c^2=\frac{A-B}{4}(J_+^2+J_-^2)+\frac{A+B}{4}(J_+J_-+J_-J_+)+CJ_z^2$

得到 $H_{rot}^{obl}=\frac{A+B}{2}J^2+(C-\frac{A+B}{2})J_z^2+\frac{A-B}{4}(J_+^2+J_-^2)$

同理 $H_{rot}^{pro}=\frac{B+C}{2}+(A-\frac{B+C}{2})J_z^2+\frac{B-C}{4}(J_+^2+J_-^2)$

$|JM\tau\rangle = \sum_{k\geq 0} a^J_{k\tau}[|JKM\rangle + (-)^\tau |J,-KM\rangle]$

不同k有混合，k不是好量子数

$V = \{E, R_a(\pi), R_b(\pi), R_c(\pi)\} \cong C_{2v}$ 克莱因四元群

C_{2v}	V	E	$R_a(\pi)$	$R_b(\pi)$	$R_c(\pi)$
A_1	A	1	1	1	1
B_1	B_a	1	1	-1	-1
A_2	B_b	1	-1	1	-1
B_2	B_c	1	-1	-1	1

$R_z(\pi)|JKM\rangle = e^{ik\pi}|JKM\rangle = (-)^k|JKM\rangle$

$R_x(\pi)|JKM\rangle = (-)^J|J,-KM\rangle \quad R_y(\pi)|JKM\rangle = (-)^J e^{-ik\pi}|J,-KM\rangle$

长陀螺极限 $a = z$

K_a	Γ^{rot}	E	R_a	R_b	R_c
0 (J even)	A	1	1	1	1
0 (J odd)	B_a	1	1	-1	-1
odd	$B_b \oplus B_c$	2	-2	0	0
even	$A \oplus B_a$	2	2	0	0

扁陀螺极限$c = z$

K_c	Γ^{rot}	E	R_a	R_b	R_c
0 (J even)	A	1	1	1	1
0 (J odd)	B_c	1	-1	-1	1
odd	$B_a \oplus B_b$	2	0	0	-2
even	$A \oplus B_c$	2	0	0	2

Fano共振

$|\psi_f\rangle = \alpha|\phi_0\rangle^a + \int \mathrm{d}E_b \beta_b |\psi_0^b\rangle$

束缚态a: $\hat{H}_0|\phi_0^a\rangle = E_a|\phi_0^a\rangle$ 连续态b: $\hat{H}_0|\phi_0^b\rangle = E_b|\phi_0^b\rangle$

$\hat{H} = \hat{H}_0 + \hat{V}, \quad \langle\phi_0^a|\hat{H}|\phi_0^a\rangle = E_a, \langle\phi_0^b|\hat{H}|\phi_0^{b'}\rangle = E_b\delta(E_{b'} - E_b), \langle\phi_0^a|\hat{H}|\phi_0^b\rangle = V_b$

$\hat{H}|\psi\rangle = E|\psi\rangle \implies \begin{cases}\alpha E_a + \int \mathrm{d}E_b\beta_b V_b = E_a \\ \alpha V_{b'}^* + \beta_{b'}E_{b'} = \beta_{b'}E\end{cases}$

Fano-Dirac Ansatz $\beta_{b'} = \frac{\alpha V_{b'}^*}{E-E_{b'}} + Z_E\delta(E-E_{b'})V_{b'}\alpha = \alpha V_{b'}^*\left[\frac{1}{E-E_{b'}} + Z_E\delta(E-E_{b'})\right]$

即$E_a + \int \mathrm{d}E_b\frac{|V_b|^2}{E-E_b} + Z_E|V_E|^2 = E$，积分项记为$F(E)$

$\implies Z_E = \frac{E-(E_a+F(E))}{|V_E|^2} = \frac{E-E_R}{\frac{\pi\Gamma}{2}} = \pi\varepsilon,\ \varepsilon = 0$共振

$\alpha=\frac{\sin\delta}{\pi V_E},\beta_{b'}=\frac{V_b}{\pi V_E}\frac{\sin\delta}{E-E_b}-\cos\delta\delta(E-E_{b'}),\tan\delta=-\frac{\pi}{2\varepsilon}$

从而 $|\psi(E)\rangle=\frac{\sin\delta}{\pi V_E}|\phi\rangle-\cos\delta\left|\phi_0^E\right\rangle,\quad|\phi\rangle=\left|\phi_0^a\right\rangle+\int\mathrm{d}E_b\frac{V_b}{E-E_b}\left|\phi_0^b\right\rangle$

$\langle\psi(E)|H|GS\rangle=-\cos\delta\left\langle\phi_0^a\right|H|GS\rangle+\frac{\sin\delta}{\pi V_E^*}\langle\phi|H|GS\rangle$

进而 $\frac{|\langle\psi(E)|H|GS\rangle|^2}{|\langle\phi_0^E|H|GS\rangle|^2}=(-\cos\delta+\frac{\sin\delta}{\pi V_E^*}\frac{\langle\phi|H|GS\rangle}{\langle\phi_0^E|H|GS\rangle})^2$，引入Fano q参数

$\frac{|\langle\psi(E)|H|GS\rangle|^2}{|\langle\phi_0^E|H|GS\rangle|^2}=(-\cos\delta+q\sin\delta)^2=\frac{(\varepsilon+q)^2}{1+\varepsilon^2},\quad\varepsilon=\frac{E-E_R}{\frac{\pi\Gamma}{2}}$