UNOFFICIAL SOLUTIONS BY TheLongCat

B3. QUANTUM, ATOMIC AND MOLECULAR PHYSICS

TRINITY TERM 2014

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Disclaimer: due to its unofficial nature, the author does not warrant the accuracy of the presented solutions in any form. However, the author is happy to discuss the typos and errors should one arises.

Turn over as you please – we are NOT under exam conditions here.

1. (DRAFT)

(a) For each e$^-$, it has energy of form $\hat{H}_i = \hat{\mathbf{p}}^2/2m - Ze^2/4\pi\epsilon_0\hat{r}_i$, where the first term is non-relativistic kinetic energy, the second being the Coulomb potential of the nucleus with atomic number Z.

Expressing $\hat{\mathbf{p}^2}$ in position representation gives $-\hbar^2\nabla^2$.

The final part, $e^2/4\pi\epsilon_0\hat{r}_{12}$, of the overal Hamiltonian is the inter-e$^-$ repulsion.

For 2 identical particles, since there is no way of distinguishing one from another, we have exchange symmetry in the system – that is a wavefunction must be an eigenfunction of the parity operator.

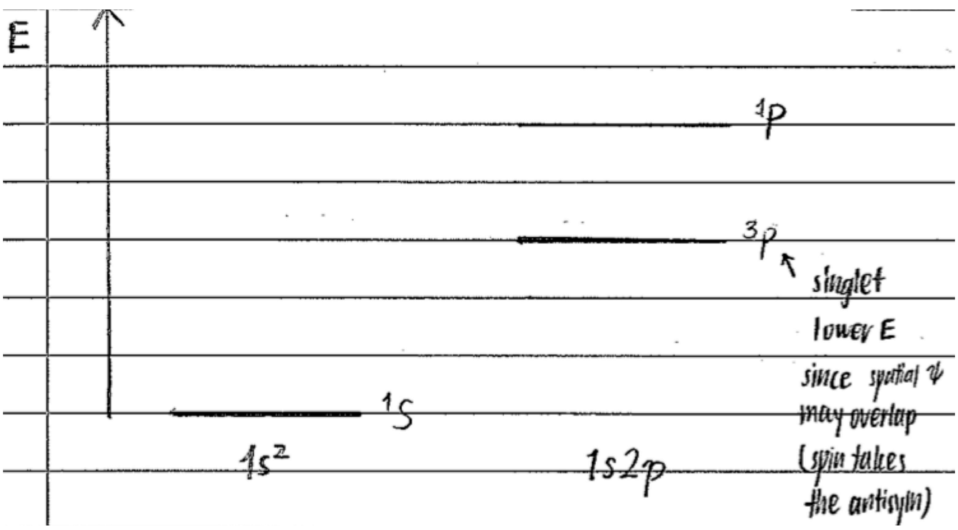
Parity operator is defined such that $\hat{\mathcal{P}}^2\psi = \psi \Rightarrow \hat{\mathcal{P}}\psi = \pm\psi$ and so the wavefunction must be either symmetric or antisymmetric.

For the $1s^2$ config, Pauli's exclusion principle tells us that two e$^-$, as fermions, could not occupy the same quantum stute, hence the wavefunction must be antisymmetric so that $\psi \to 0$ as the e$^-$ draws close.

For the $1s2p$ config, since the e$^-$ occupy different orbitals, Pauli's exclusion principle does not apply and thus the wavefunction may be either symmetric or antisymmetric.

The nature of fermions being antisymmetric also mandates that the spin wavefunction must be symmetric ($S = 1$) for antisymmetric spatial ψ, antisymmetric ($S = 0$) for symmetric spatial ψ.

Energy diagram of $1s^2$ and $1s2p$ config of He:



(b) **(TO EXPAND)** As Z increases, the expectation value of $1/r_{12}$ should decrease as the system increasingly pulls the e$^-$ more, making e$^-$ at different orbitals more far away.

Modelling IE as $aZ^2 + b$:

$$\Rightarrow a = 11.89\,\text{eV}$$
$$b = -21.75\,\text{eV}$$

So Al^{11+} should have IE 1952 eV, Al^{12+} should have IE given by Rydberg level:

$$\begin{aligned} E &= \frac{hcR_\infty}{1^2} \cdot Z^2 \\ &= 2300\,\mathrm{eV} \end{aligned}$$

From g to a, $\begin{array}{rcc} \text{g: } \mathrm{Al}^{12+} & \text{d: } \mathrm{Al}^{11+} & \text{a:} \\ \text{f: } \mathrm{Al}^{11+} & \text{c:} & \\ \text{e: } \mathrm{Al} & \text{b:} & \end{array}$

h is *bremsstrahlung*?

2. (DRAFT)

(a) In a many e$^-$ system, we have Hamiltonian:

$$\hat{H} = \sum_i \left[\frac{\hat{\mathbf{p}}_i^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 \hat{r}_i} + \sum_{j>i} \frac{e^2}{4\pi\epsilon_0 \hat{r}_{ij}} \right]$$

To account for the inter-e$^-$ repulsion, introduce central potential $S(r_i)$ such that $\hat{H} = \hat{H}_{\mathrm{CF}} + \Delta\hat{H}_{\mathrm{RE}}$ where:

$$\hat{H}_{\mathrm{CF}} = \sum_i \left[\frac{\hat{\mathbf{p}}_i^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 \hat{r}_i} + S(r_i) \right]$$
$$\Delta\hat{H}_{\mathrm{RE}} = \sum_i \left[\sum_{j>i} \frac{e^2}{4\pi\epsilon_0 \hat{r} ij} - S(r_i) \right]$$

Under this central field approximation, we may perturb the eigenstates of $\hat{H}_{\mathrm{CF}}$ (which forms config) with $\Delta\hat{H}_{\mathrm{RE}}$ to get a new set of eigenstates.

Since $\Delta\hat{H}_{\mathrm{RE}}$ is an internal interaction, L is a constant of motion (so is S), giving rise to the LS coupling scheme – labelling of eigenstates with $|LSM_LM_S\rangle$.

For a electric dipole transition, we have the following selection rules:

$$\text{Configuration} \begin{cases} \text{only 1 e}^- \text{ transits} \\ \Delta n = \text{any} \\ \Delta l = \pm 1 \end{cases} \quad (1) \qquad \text{Term} \begin{cases} \Delta L = 0, \pm 1 (0 \nrightarrow 0) \\ \Delta S = 0 \end{cases} \quad (2)$$

External magnetic Hamiltonian:

$$\begin{aligned} \Delta\hat{H}_z &= -\boldsymbol{\mu} \cdot \mathbf{B} \\ &= \mu_{\mathrm{B}} \mathbf{L} \cdot \mathbf{B} + g_s \mu_{\mathrm{B}} \mathbf{S} \cdot \mathbf{B} \end{aligned}$$

where $\boldsymbol{\mu} = \underbrace{\boldsymbol{\mu}_L}_{\substack{\text{orbital} \\ \text{angular} \\ \text{momentum}}} + \underbrace{\boldsymbol{\mu}_S}_{\substack{\text{spin} \\ \text{angular} \\ \text{momentum}}} = -\mu_{\mathrm{B}} \mathbf{L} - g_s \mu_{\mathrm{B}} \mathbf{S}$.

By Wigner-Eckart Theorem,

$$\mathbf{L} \cdot \mathbf{B} \to \frac{\mathbf{L} \cdot \mathbf{J}}{J^2} \mathbf{J} \cdot \mathbf{B}$$
$$\mathbf{S} \cdot \mathbf{B} \to \frac{\mathbf{S} \cdot \mathbf{J}}{J^2} \mathbf{J} \cdot \mathbf{B}$$

Hence:

$$\Delta\hat{H}_z = \mu_{\mathrm{B}} \frac{L^2 + \mathbf{L} \cdot \mathbf{S} + g_s S^2 + g_s \mathbf{S} \cdot \mathbf{L}}{J^2} \mathbf{J} \cdot \mathbf{B}$$
$$\Rightarrow \Delta E_z = g_J \mu_{\mathrm{B}} B M_J$$

where:

$$g_J = \frac{\begin{aligned} L(L+1) + \frac{1}{2}[J(J+1) - L(L+1) - S(S+1)] \\ + g_s S(S+1) + \frac{g_s}{2}[J(J+1) - L(L+1) - S(S+1)] \end{aligned}}{J(J+1)}$$

Approximating $g_s \simeq 2$:

$$\begin{aligned} g_J &= \frac{\begin{aligned} \cancel{2L(L+1)} + J(J+1) - L(L+1) - S(S+1) + \cancel{2S(S+1)} \\ + 2J(J+1) \cancel{-2L(L+1)} \cancel{-2S(S+1)} \end{aligned}}{2J(J+1)} \\ &= \frac{3}{2} - \frac{L(L+1) + S(S+1)}{2J(J+1)} \end{aligned}$$

(b) For Zeeman transitions, we have selection rules:

$$\text{Level} \begin{cases} \Delta J = 0, \pm 1 (0 \nrightarrow 0) \\ \Delta M_J = 0, \pm 1 (0 \nrightarrow 0 \iff \Delta J = 0) \end{cases}$$

"Weak" magnetic flux refers to the requirement that $\Delta \hat{H}_z \ll \underbrace{\Delta \hat{H}_{\text{SO}}}_{\substack{\text{spin-orbit} \\ \text{interaction}}}$.

$$\Rightarrow g_J \mu_B B M_J \ll \beta_{\text{SO}} \cdot \frac{1}{2} [J(J+1) - L(L+1) - S(S+1)]$$

(c) Alkali has 1 valence e^-, and that $\Delta S = 0 \Rightarrow S_1 = S_2 = 1/2$

$\Rightarrow J_2$ should be in between 3/2 and 5/2

$J_2 > J_1$ so L_1 must be $2 - 1 = 1 \Rightarrow$ possible J_1 value: 1/2, 3/2

The only consistent set with $\Delta J = 0, \pm 1$ would be $J_2 = 3/2$, $J_1 = 1/2$ since $J_2 > J_1$.

For upper level, $^2D_{3/2}$:

$$\begin{aligned} g_J &= \frac{3}{2} - \frac{2(3) + \frac{1}{2}\left(\frac{3}{2}\right)}{2\left(\frac{3}{2}\right)\left(\frac{5}{2}\right)} \\ &= \frac{9}{10} \end{aligned}$$

So:

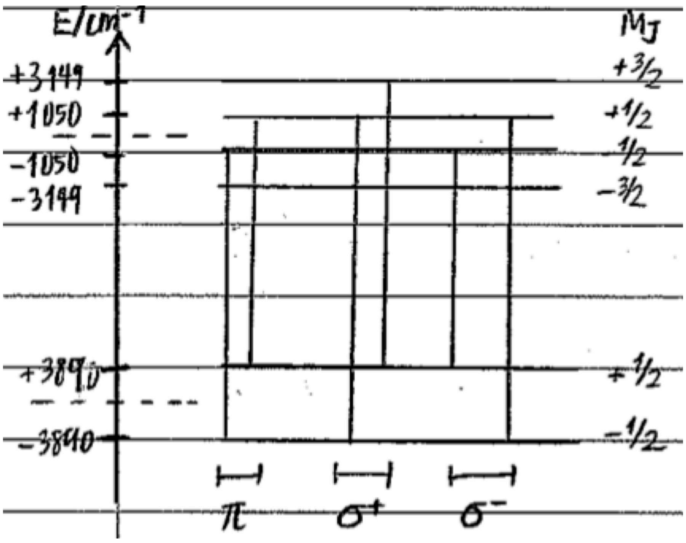
$$\begin{aligned} \Delta E &= g_J \mu_B B M_J \\ &= \begin{cases} \pm 31.49\,\text{m}^{-1} & M_J = \pm\frac{3}{2} \\ \pm 10.50\,\text{m}^{-1} & M_J = \pm\frac{1}{2} \end{cases} \end{aligned}$$

For lower level, $^2P_{1/2}$:

$$g_J = \frac{3}{2} - \frac{1(2) + \frac{1}{2}\left(\frac{3}{2}\right)}{2\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)}$$
$$= -\frac{1}{3}$$

So:

$$\Delta E = \mp 3.89\,\mathrm{m}^{-1} \qquad M_J = \pm\frac{1}{2}$$



π and σ's are visible perpendicular to B.

Only σ's are visible parallel to B.

3. **(DRAFT)**

(a) $\alpha = e^2/4\pi\epsilon_0 \hbar c$ represents the scale of the $1/r$ potential in the Bohr model: $V(r) = \alpha\hbar c/r$.

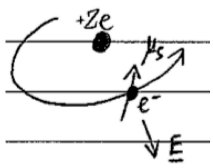
$$\begin{aligned}\frac{\alpha^2 m_e c^2}{2} &= \frac{0.511\,\text{eV}}{2\cdot 137.04^2} \\ &= 1.360\times 10^{-5}\,\text{MeV} \\ &= 13.60\,\text{eV}\end{aligned}$$

This is simply the ground state of the e$^-$ in hydrogen.

Relativistic Hamiltonian:

$$\begin{aligned}\hat{H} &= \sqrt{m_e^2c^4 + \hat{p}^2c^2} - m_ec^2 + V(r) \\ &= m_ec^2\left[1 + \frac{1}{2}\frac{\hat{p}^2}{m_e^2c^2} + \mathcal{O}\left(\frac{\hat{p}^4}{m_e^4c^4}\right)\right] - m_ec^2 + V(r) \\ &= \frac{\hat{p}^2}{2m_e} + V(r) + \mathcal{O}\left(\frac{\hat{p}^4}{m_e^4c^4}\right)\end{aligned}$$

Since the ground state gross structure $\propto \alpha^2$, I then expect fine structure to be proportional to $(\alpha^2)^2 = \alpha^4$.



(b) In e$^-$ rest frame,

$$\begin{aligned}\mathbf{B} &= -\frac{\mathbf{v}\times\mathbf{E}}{c^2} \\ &= -\frac{1}{m_ec^2}\,\mathbf{p}\times\left(+\frac{1}{e}\frac{\partial V}{\partial r}\frac{\mathbf{r}}{r}\right) \\ &= \frac{1}{m_ec^2}\left(\frac{1}{er}\frac{\partial V}{\partial r}\right)\hbar\mathbf{l}\end{aligned}$$

since $\mathbf{r}\times\mathbf{p} = \hbar\mathbf{l}$.

Spin-orbit Hamiltonian:

$$\begin{aligned}\Delta\hat{H}_{\text{SO}} &= -\boldsymbol{\mu}_s\cdot\mathbf{B} \\ &= g_s\mu_{\text{B}}\mathbf{s}\cdot\frac{1}{m_ec^2}\left(\frac{1}{er}\frac{\partial V}{\partial r}\right)\hbar\mathbf{l}\end{aligned}$$

Thomas precession tells us $g_s \to g_s - 1 \simeq 1$ so:

$$\begin{aligned}\Delta\hat{H}_{\text{SO}} &= \frac{e\hbar}{2m_e}\cdot\frac{\hbar}{m_ec^2}\left(\frac{1}{er}\frac{\partial V}{\partial r}\right)\mathbf{s}\cdot\mathbf{l} \\ &= \frac{1}{2m_e^2c^2}\left(\frac{1}{r}\frac{\partial V}{\partial r}\right)\mathbf{l}\cdot\mathbf{s}\end{aligned}$$

setting $\hbar = 1$.

(c) For hydrogenic ions,

$$
\begin{aligned}
V(r) &= -\frac{Ze^2}{4\pi\epsilon_0 r} \\
\Rightarrow \frac{1}{r}\frac{\partial V}{\partial r} &= \frac{Ze^2}{4\pi\epsilon_0 r^3}
\end{aligned}
$$

$$
\begin{aligned}
\Delta E_{\text{SO}} &= \frac{1}{2m_e^2c^2}\cdot\frac{Ze^2}{4\pi\epsilon_0}\underbrace{\left\langle\frac{1}{r^3}\right\rangle}_{\substack{\frac{1}{81}\left(\frac{Z}{a_0}\right)^3 \\ \text{for } 3p}}\underbrace{\langle\mathbf{l}\cdot\mathbf{s}\rangle}_{\frac{1}{2}[j(j+1)-l(l+1)-s(s+1)]} \\
&= \frac{Ze^2}{1296m_e^2c^2\cdot\pi\epsilon_0}\left(\frac{Z}{a_0}\right)^3[j(j+1)-l(l+1)-s(s+1)]
\end{aligned}
$$

For $3p$ e^-, $l=1$, $s=1/2$:

$$
\begin{aligned}
E_{3/2}-E_{1/2} &= \frac{Z^4e^2}{1296\pi\epsilon_0 m_e^2c^2}\frac{1}{a_0}\left[\frac{3}{2}\left(\frac{5}{2}\right)\cancel{-1(2)-\frac{1}{2}\left(\frac{3}{2}\right)}-\frac{1}{2}\left(\frac{3}{2}\right)\cancel{+1(2)-\frac{1}{2}\left(\frac{3}{2}\right)}\right] \\
&= \frac{Z^4e^2}{432\pi\epsilon_0 m_e^2c^2}\cdot\left(\frac{m_ee^2}{4\pi\epsilon_0\hbar^2}\right)^3 \\
&= \frac{Z^4e^8m_e}{432\pi^4\epsilon_0^4c^2} \\
&= \frac{Z^4m_e}{432c^2}\left(\frac{e^2}{4\pi\epsilon_0 c}\right)^4\cdot 4^4c^4 \\
&= \frac{1}{108}(Z\alpha)^4 m_ec^2
\end{aligned}
$$

For hydrogen, $Z=1$:

$$
\begin{aligned}
E_{3/2}-E_{1/2} &= \frac{1}{108}\alpha^4m_ec^2 \\
&= \frac{0.511\,\text{MeV}}{108\cdot 137.04^4} \\
&= 1.342\times10^{-11}\,\text{MeV} \\
&= 1.342\times10^{-5}\,\text{eV} \\
&= 67.985\,\text{m}^{-1}
\end{aligned}
$$

Empirical $E_{3/2}-E_{1/2}$:

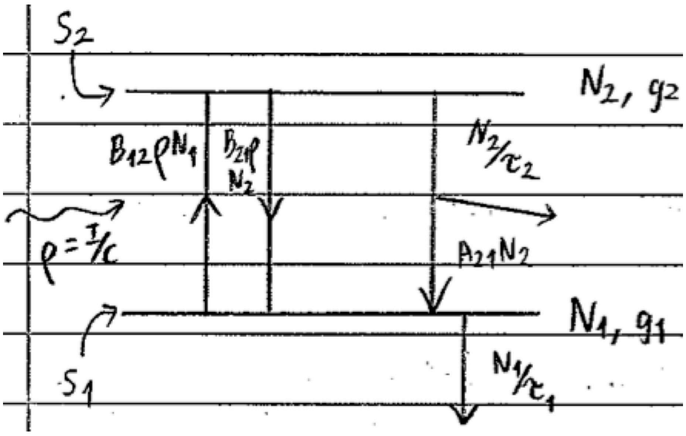
$$
\begin{aligned}
\delta E &= \left|hc\left[\frac{1}{589.6\,\text{nm}}-\frac{1}{589.0\,\text{nm}}\right]\right| \\
&= 1727.74\,\text{m}^{-1} \\
&= 2.142\times10^{-9}\,\text{MeV}
\end{aligned}
$$

Equate $\delta E = 1/108(Z\alpha)^4 m_e c^2$:

$$\begin{aligned}\Rightarrow Z^4 &= \frac{108\delta E}{\alpha^4 m_e c^2} \\ &= 159.68 \\ \Rightarrow Z_{\text{eff}} &= 3.55\end{aligned}$$

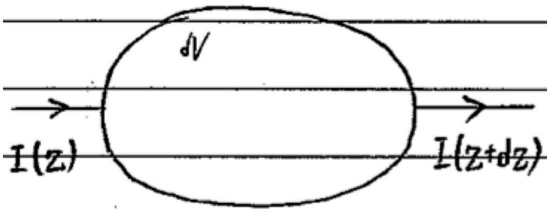
The effective Z is smaller than the actual Z since the valence e$^-$ experiences shielding by the core e$^-$, thereby experiencing lower effective Z.

4. (DRAFT)



(a) Rate equations:

$$\frac{\mathrm{d}N_2}{\mathrm{d}t} = S_2 + B_{12}\rho N_1 - B_{21}\rho N_2 - \frac{N_2}{\tau_2}$$
$$\frac{\mathrm{d}N_1}{\mathrm{d}t} = S_1 + B_{21}\rho N_2 - B_{12}\rho N_1 + A_{21}N_2 - \frac{N_1}{\tau_1}$$



Change in number of photons due to the radiative process:

$$\Delta N_\gamma = [B_{21}\rho N_2 - B_{12}\rho N_1]\underbrace{\mathrm{d}V}_{A\,\mathrm{d}z}$$
$$= B_{21}\rho\left(N_2 - \frac{g_2}{g_1}N_1\right)A\,\mathrm{d}z$$

since $g_1 B_{12} = g_2 B_{21}$.

Change in beam energy:

$$\Delta E = \Delta N_\gamma \cdot \hbar\omega$$
$$= [I(z + \mathrm{d}z) - I(z)]\,A\,\mathrm{d}\omega$$

$$\Rightarrow \frac{B_{21}\left(N_2 - \frac{g_2}{g_1}N_1\right)I\hbar\omega}{c} g_{\mathrm{H}}\cancel{A}\,\mathrm{d}z\,\cancel{\mathrm{d}\omega} = \mathrm{d}I\cancel{A}\,\cancel{\mathrm{d}\omega}$$
$$\frac{\mathrm{d}I}{\mathrm{d}z} = \underbrace{\left(N_2 - \frac{g_2}{g_1}N_1\right)}_{N^*}\underbrace{B_{21}g_{\mathrm{H}}\frac{\hbar\omega}{c}}_{\sigma_{21}}I$$

where a transformation $\rho \to \rho g_{\mathrm{H}}$ was made to take into account of narrowband broadening.

Now rewrite the rate equations with N^* and σ:

$$\frac{\mathrm{d}N_2}{\mathrm{d}t} = S_2 - B_{21}\rho g_{\mathrm{H}}\delta\omega N^* - \frac{N_2}{\tau_2}$$
$$\frac{\mathrm{d}N_1}{\mathrm{d}t} = S_1 + B_{21}\rho g_{\mathrm{H}}\delta\omega N^* + A_{21}N_2 - \frac{N_1}{\tau_1}$$

At steady state, ${}^{\mathrm{d}N_2}/_{\mathrm{d}t} = {}^{\mathrm{d}N_1}/_{\mathrm{d}t} = 0$, so:

$$\begin{aligned}
N_2 &= S_2\tau_2 - B_{21}\rho g_{\mathrm{H}}\delta\omega N^*\tau_2 \\
N_1 &= S_1\tau_1 + B_{21}\rho g_{\mathrm{H}}\delta\omega N^*\tau_1 + A_{21}N_2\tau_1 \\
&= S_1\tau_1 + B_{21}\rho g_{\mathrm{H}}\delta\omega N^*\tau_1 + A_{21}\left[S_2\tau_2 - B_{21}\rho g_{\mathrm{H}}\delta\omega N^*\tau_2\right]\tau_1
\end{aligned}$$

So:

$$\begin{aligned}
N^* &= N_2 - \frac{g_2}{g_1}N_1 \\
&= S_2\tau_2 - B_{21}\rho g_{\mathrm{H}}\delta\omega N^*\tau_2 \\
&\quad - \frac{g_2}{g_1}\left[S_1\tau_1 + B_{21}\rho g_{\mathrm{H}}\delta\omega N^*\tau_1 + A_{21}\tau_1\left(S_2\tau_2 - B_{21}\rho g_{\mathrm{H}}\delta\omega N^*\tau_2\right)\right] \\
&= S_2\tau_2 - \frac{g_2 A_{21}\tau_1}{g_1}S_2\tau_2 - \frac{g_2 S_1\tau_1}{g_1} \\
&\quad - \frac{\sigma_{21}}{\hbar\omega}I\left[N^*\tau_2 + \frac{g_2}{g_1}N^*\tau_1 - \frac{g_2}{g_1}A_{21}\tau_1 N^*\tau_2\right] \\
\Rightarrow N^*(I) &= \frac{N^*(0)}{1 + \dfrac{I}{I_s}}
\end{aligned}$$

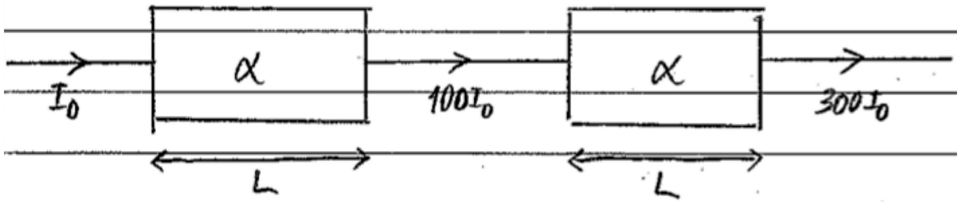
where:

$$N^*(0) = S_2\tau_2\left[1 - \frac{g_2 A_{21}\tau_1}{g_1}\right] - \frac{g_2}{g_1}S_1\tau_1$$
$$I_s = \frac{\hbar\omega}{\sigma_{21}}\left[\tau_2 + \frac{g_2}{g_1}\tau_1 - \frac{g_2}{g_1}A_{21}\tau_1\tau_2\right]^{-1}$$

(b) Recall that the definition of beam gain coefficient:

$$\alpha = N^*\sigma_{21}$$
$$\alpha(I) = \frac{N^*(0)\sigma_{21}}{1 + \dfrac{I}{I_s}}$$

The reason why the input signal level affects beam gain has to do with the fact that lasing burns out population inversion – as the intensity of a beam grows, the inversion begins to burn out more, reducing gain. This of course warrants the assumption of thermal equilibrium, which implicitly assumes that we are looking at continuous operation. Pulsed laser may be possible even if inversion is impossible in equilibrium.



Beam growth equation:

$$\begin{aligned}
\frac{\mathrm{d}I}{\mathrm{d}z} &= \alpha I \\
\Rightarrow \frac{\mathrm{d}I}{\mathrm{d}z} &= \frac{\alpha(0)}{1+\dfrac{I}{I_s}} I \\
\Rightarrow \frac{1}{I} + \frac{1}{I_s}\,\mathrm{d}I &= \alpha(0)\,\mathrm{d}z \\
\Rightarrow \ln\left(\frac{I}{I_0}\right) + \frac{I - I_0}{I_s} &= \alpha(0)L
\end{aligned}$$

Since the amplifiers are identical,

$$\begin{aligned}
\ln\left(\frac{100I_0}{I_0}\right) + \frac{100I_0 - I_0}{I_s} &= \ln\left(\frac{300I_0}{100I_0}\right) + \frac{300I_0 - I_0}{I_s} \\
\Rightarrow \frac{200I_0}{I_s} &= \ln(100) - \ln(3) \\
I_s &= \frac{200I_0}{\ln(100) - \ln(3)} \\
&= 57.0I_0
\end{aligned}$$