

Some Quick and Dirty Comments About Polarizing Xe-129

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Abstract

Simple scaling formulas are derived for estimating the minimum power required to polarize amagat levels of Xe-129 using the FEL tuned to the D1 transition of Cesium. If it ever happens, Version 2.0 will contain the results of a numerical simulation.

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1 Rate Equations

The general rate equations for the polarizations for single alkali-Xe SEOP are given by:

$$\frac{dP_A}{dt} = +A_1 - A_2/2 - A_0P_A + k_{se}[129](P_{129} - P_A) + k'_{se}[131](P_{131} - P_A) - \Gamma_A P_A \quad (1)$$

$$\frac{dP_{129}}{dt} = +k_{se}[A](P_A - P_{129}) - \Gamma_{129}P_{129} \quad (2)$$

$$\frac{dP_{131}}{dt} = +k'_{se}[A](P_A - P_{131}) - \Gamma_{131}P_{131} \quad (3)$$

where P is the polarization of a particular species, $A_{(1,2)}$ is the differential D1 (D2) optical pumping rate, A_0 is the total optical pumping rate, $k_{se}(k'_{se})$ is the spin-exchange rate constant for Xe-129 (Xe-131), $[\dots]$ refer to a number density, Γ is the relaxation rate of a particular species, and the symbols/subscripts A, 129, 131 specify the alkali metal, Xe-129, & Xe-131 respectively. The optical pumping rates are defined by:

$$A_0 = 2\Lambda \int_0^\infty [\Phi_{\mathcal{R}}(\nu, \vec{r}) + \Phi_{\mathcal{L}}(\nu, \vec{r})] [\sigma_1^A(\nu) + \sigma_2^A] d\nu \quad (4)$$

$$A_1 = 2\Lambda \int_0^\infty [\Phi_{\mathcal{R}}(\nu, \vec{r}) - \Phi_{\mathcal{L}}(\nu, \vec{r})] \cos(\theta) \sigma_1^A(\nu) d\nu \quad (5)$$

$$A_2 = 2\Lambda \int_0^\infty [\Phi_{\mathcal{R}}(\nu, \vec{r}) - \Phi_{\mathcal{L}}(\nu, \vec{r})] \cos(\theta) \sigma_2^A(\nu) d\nu \quad (6)$$

where Λ is the fraction of alkali atoms in the excited state that return to the opposite ground state, $\Phi_{\mathcal{R}(\mathcal{L})}$ is the photon flux for right (left) circularly polarized light, θ is the angle between the magnetic field & the laser beam direction, $\sigma_{1(2)}^A$ is the unpolarized absorption cross section for D1 (D2) transitions. The following equations account for attenuation of the photon flux as the beam propagates through the cell along the z direction:

$$\frac{d\Phi_{\mathcal{R}}}{dz} = - \left((1 - P_A \cos(\theta)) \sigma_1^A + \left(1 + \frac{P_A}{2} \cos(\theta) \right) \sigma_2^A \right) [A] \Phi_{\mathcal{R}} \quad (7)$$

$$\frac{d\Phi_{\mathcal{L}}}{dz} = - \left((1 + P_A \cos(\theta)) \sigma_1^A + \left(1 - \frac{P_A}{2} \cos(\theta) \right) \sigma_2^A \right) [A] \Phi_{\mathcal{L}} \quad (8)$$

At equilibrium, the polarizations are obtained by setting the previous equations to zero:

$$P_A = \frac{A_1 - A_2/2}{A_0 + k_{\text{se}}[129] \left(1 - \frac{P_{129}}{P_A} \right) + k'_{\text{se}}[131] \left(1 - \frac{P_{131}}{P_A} \right) + \Gamma_A} \quad (9)$$

$$\frac{P_{129}}{P_A} = \frac{k_{\text{se}}[A]}{k_{\text{se}}[A] + \Gamma_{129}} \quad (10)$$

$$\frac{P_{131}}{P_A} = \frac{k'_{\text{se}}[A]}{k'_{\text{se}}[A] + \Gamma_{131}} \quad (11)$$

where unbalanced spin exchange between the alkali metal and Xe acts as an effective relaxation mechanism for the alkali metal:

$$\Gamma'_A = \Gamma_A + k_{\text{se}}[129] \left(1 - \frac{P_{129}}{P_A} \right) + k'_{\text{se}}[131] \left(1 - \frac{P_{131}}{P_A} \right) = \Gamma_A + \left(\frac{k_{\text{se}}[129]}{k_{\text{se}}[A] + \Gamma_{129}} \right) \Gamma_{129} + \left(\frac{k'_{\text{se}}[131]}{k'_{\text{se}}[A] + \Gamma_{131}} \right) \Gamma_{131} \quad (12)$$

2 Assumptions & Rate Constants

1. The polarization time scale for an alkali atom is much shorter than it's diffusion timescale. Therefore, the alkali polarization is sensitive to the local light polarization and intensity.
2. The polarization time scale for a Xe atom is on order of it's diffusion timescale. However, we'll make the same argument that we made for the alkali atoms. Therefore, the Xe polarization is sensitive to the local alkali polarization.
3. We'll ignore the possibility that there are both an extra alkali relaxation rate that scales with the optical pumping rate and an extra Xe relaxation rate that scales with the alkali density. In the language of He-3 SEOP, this implies $X_A = X = 0$.
4. Since we're considering Rb (795 nm vs. 780 nm) and Cs (894 nm vs. 852 nm), we'll ignore the possibility of optical pumping the D2 line because it is so far away in both cases, $A_2/A_1 \ll 1$. In addition, we'll assume that the skew angle is zero, $\cos(\theta) = 1$, and that the light polarization is 1, $\Phi_{\mathcal{L}} = 0$. All this together implies that $A_0 = A_1 = A$ and $\Phi_{\mathcal{R}} = \Phi$.
5. We'll assume that an excited alkali atom has an equal probability of returning to either ground state, so $2\Lambda = 1$.
6. We'll assume that the emission spectrum is centered on the absorption spectrum, so $\nu_0 = \nu_n$.
7. We'll assume that the Xe-129 relaxation is dominated by wall relaxation.
8. We'll assume that we're using 0.2 amg of N_2 and 1-10 amagats of isotopically enriched Xe: Xe-129 (80%) & Xe-131 (20%). In addition, we'll assume a 2.0 inch diameter cell, which results in about 50 to 500 cc · atm of Xe-129.

Species	Reaction	rate constant	units	reference
Rb	relaxation by Rb	0.065	kHz per $10^{14}/\text{cm}^3$	Knize
Rb	relaxation by Cs	0.21	kHz per $10^{14}/\text{cm}^3$	geometric mean
Rb	relaxation by N_2	0.25	kHz per amg	Wagshul/Chupp
Rb	binary exchange w/ Xe-131	1	kHz per amg	Ishy priv comm
Rb	3-body exchange w/ Xe-131	3	kHz · amg per amg	Ishy priv comm
Rb	binary exchange w/ Xe-129	10	kHz per amg	Cates 1992
Rb	relaxation by Xe	18	kHz per amg	some ref Ishy
Rb	3-body exchange w/ Xe-129	30	kHz · amg per amg	Cates 1992
Cs	relaxation by Rb	0.21	kHz per $10^{14}/\text{cm}^3$	geometric mean
Cs	relaxation by N_2	0.25	kHz per amg	est by Rb
Cs	relaxation by Cs	0.7	kHz per $10^{14}/\text{cm}^3$	Bhaskar
Cs	binary exchange w/ Xe-131	1.1	kHz per amg	Ishy priv comm
Cs	3-body exchange w/ Xe-131	3	kHz · amg per amg	est by Rb
Cs	binary exchange w/ Xe-129	11	kHz per amg	Jau 2004
Cs	relaxation by Xe	18	kHz per amg	est by Rb
Cs	3-body exchange w/ Xe-129	30	kHz · amg per amg	est by Rb
A	exchange w/ A	90	kHz per $10^{14}/\text{cm}^3$	OP72
Xe-129	relaxation by Xe	0.005	mHz per amg	RMP97
Xe-131	binary exchange w/ Rb	3.7	mHz per $10^{14}/\text{cm}^3$	Ishy priv comm
Xe-131	binary exchange w/ Cs	4.1	mHz per $10^{14}/\text{cm}^3$	Ishy priv comm
Xe	relaxation due to the wall	1 to 10	mHz	James' Thesis
Xe-131	3-body exchange w/ A	11	mHz · amg per $10^{14}/\text{cm}^3$	Ishy priv comm
Xe-129	binary exchange w/ Rb	37	mHz per $10^{14}/\text{cm}^3$	Cates 1992
Xe-131	relaxation by Xe	40	mHz per amg	RMP97
Xe-129	binary exchange w/ Cs	41	mHz per $10^{14}/\text{cm}^3$	Jau 2004
Xe-129	3-body exchange w/ A	110	mHz · amg per $10^{14}/\text{cm}^3$	Cates 1992

Table 1: Rate Constants for Spin Exchange and Spin Relaxation. When rate constant data is unavailable, we'll use the Rb value or scale by the ratio of the square of the Xe nuclear gyromagnetic ratios.

9. We'll assume that the laser beam spot can be modeled by gaussian beam optics.
10. We'll assume a laser power of up to 2 kW with a spectral emission linewidth as low as FWHM = 150 GHz.
11. We'll ignore the satellite lines (or "shoulder") in the pressure broadened absorption spectrum of that alkali metal that is due to molecular formation with Xe.

3 Binary and Three Body Spin Exchange Rates

The spin exchange rate constant for Xe is usually given as a sum of two parts:

$$k_{se} = \left(\langle \sigma v \rangle_2 + \frac{\gamma_M \zeta}{[\text{Xe}]} \right) = \langle \sigma v \rangle_2 \left(1 + \frac{[\text{Xe}]_3}{[\text{Xe}]} \right) \quad (13)$$

where $\langle \sigma v \rangle_2$ is the binary spin exchange rate constant, γ_M is the three body van der Waals rate constant, ζ is a unitless parameter that accounts for the effect of the alkali nuclear spin during spin exchange, and $[\text{Xe}]_3$

isotope	nat. abund., f_i	nuclear spin, I	paramagnetic coefficient, $\epsilon(I, P)$
Rb-85	0.7217	5/2	$(35 + 42P^2 + 3P^4) / (3 + 10P^2 + 3P^4)$
Rb-87	0.2783	3/2	$(5 + P^2) / (1 + P^2)$
Cs-133	1.0	7/2	$(21 + 63P^2 + 27P^4 + P^6) / (1 + 7P^2 + 7P^4 + P^6)$

Table 2: Rb and Cs Nuclear Data

alkali species	ζ for $P_A = 0$	$[\text{Xe}]_3$ for $P_A = 0$	ζ for $P_A = 1$	$[\text{Xe}]_3$ for $P_A = 1$
Rb	0.1791	0.53 amg	0.0949	0.28 amg
Cs	$11/64 = 0.1719$	0.50 amg	$1/16 = 0.0625$	0.18 amg

Table 3: ζ values for natural abundance Rb and Cs at high and low alkali polarizations. Also listed is the Xe density $[\text{Xe}]_3$ for which the binary and three body spin exchange rates are equal.

is the Xe density for which the binary and three body rates are equal. The term ζ depends on the alkali polarization through the paramagnetic coefficient $\epsilon(I, P_A)$ and is given by:

$$\zeta = \frac{1}{2} \sum_i \frac{f_i (1 + \epsilon(I_i, P_A))}{(2I_i + 1)^2} \quad (14)$$

where I_i & f_i are respectively the nuclear spin & fraction of alkali species i . Typical values of ζ are give in table blah, but the bottom line is that for densities of much more than 1/2 an amagat of Xe, binary spin exchange dominates.

One final note is how we calculate the Xe-131 rates since we can not find them in the literature. Since the electronic wavefunctions of Xe-129 and Xe-131 are identical, the spin exchange matrix element scales only with the gyromagnetic ratio. Therefore the cross section should scale as a the square of the gyromagnetic ratios, ignoring the small difference in thermal velocities (private communication with “Urinate Pants If Hot”):

$$\frac{k'_{\text{se}}}{k_{\text{se}}} = \frac{\sigma'_{\text{se}}}{\sigma_{\text{se}}} = \frac{|\langle M'_{\text{se}} \rangle|^2}{|\langle M_{\text{se}} \rangle|^2} = \left| \frac{\gamma_{131}}{\gamma_{129}} \right|^2 \approx 0.1 \quad (15)$$

4 Optical Pumping Rates

The photon absorption cross section $\sigma(\nu)$ is given by:

$$\sigma_n^A(\nu) = \pi f_n r_e c L(\nu) \quad (16)$$

where f_n is the oscillator strength (1/3 for D1, 2/3 for D2), r_e is the classical electron radius, c is the speed of light in a vacuum, and the Lorentzian line shape $L(\nu)$ is defined such that:

$$L(\nu) = \frac{\Gamma_n/2\pi}{(\nu - \nu_n)^2 + \Gamma_n^2/4} \quad \lim_{(\Gamma_n/\nu_n) \rightarrow 0} \int_0^\infty L(\nu) d\nu = 1 \quad (17)$$

The location of the peak and it's pressure broadened width are labeled by ν_n and Γ_n (≈ 20 GHz/amg) respectively. Under our conditions, $\frac{\Gamma_n}{\nu_n} = \frac{150 \text{ GHz}}{10^5 \text{ GHz}} \approx 10^{-4} \approx 0$, so the Lorentzian lineshape has unit normalization.

The incident photon flux is defined in the following way:

$$\Phi(\nu, r, 0) = \frac{\text{number of photons}}{\text{unit cross sectional area} \times \text{unit time} \times \text{unit frequency interval}} = \phi(r, 0)G(\nu) \quad (18)$$

FWHM/Γ_n	\mathcal{L}	$\mathcal{L}\sqrt{\pi \log(2)}\Gamma_n/\text{FWHM}$
1/32	0.021	0.999
1/16	0.042	0.997
1/8	0.084	0.989
1/4	0.163	0.960
1/2	0.297	0.875
1	0.478	0.705
2	0.661	0.488
4	0.803	0.296
8	0.893	0.165
16	0.944	0.087
32	0.971	0.045
64	0.985	0.023
128	0.993	0.011
256	0.996	0.006
512	0.998	0.003
1024	0.999	0.001

Table 4: Lineshape parameter vs. emission linewidth to absorption linewidth ratio. For ratios smaller than about 1/3, the emission spectrum looks like a delta function. For ratios larger than about 8, the absorption spectrum looks like a delta function. In between, it's necessary to obtain the value by a numerical integration.

where the Gaussian lineshape $G(\nu)$ is defined by:

$$G(\nu) = \frac{2\sqrt{\log(2)}/\pi}{\text{FWHM}} \exp\left(-4\log(2)\frac{(\nu - \nu_0)^2}{\text{FWHM}^2}\right) \quad \lim_{\left(\frac{\text{FWHM}}{\nu_0}\right) \rightarrow 0} \int_0^\infty G(\nu) d\nu = 1 \quad (19)$$

Under our conditions, $\frac{\text{FWHM}}{\nu_0} = \frac{150 \text{ GHz}}{10^9 \text{ GHz}} \approx 10^{-4} \approx 0$, so the Gaussian lineshape also has unit normalization. Assuming the fundamental gaussian mode, which implies cylindrical symmetry, ϕ has a radial dependence at the front of the cell that is given by:

$$\phi(r) = \frac{P_0}{h\nu_0} \frac{2}{w^2\pi} \exp\left(-\frac{2r^2}{w^2}\right) \quad \int_0^\infty 2\pi r h\nu_0 \phi(r) dr = P_0 \quad (20)$$

where P_0 is the total power of the beam, h is Planck's constant, ν_0 is the center frequency of emission spectrum, w is the beam radius, and r is the radial distance from the center of the beam spot. Putting all this together gives the following for the optical pumping rate at the front of the cell:

$$A(r, 0) = \int_0^\infty \Phi(\nu, r, 0) \sigma(\nu) d\nu = \frac{2P_0(r)f_n r_e \lambda_0}{hw^2} \int_0^\infty L(\nu) G(\nu) d\nu \quad (21)$$

Since the emission linewidth is rarely smaller than the absorption linewidth, it's useful to define a unitless lineshape parameter \mathcal{L} as:

$$\mathcal{L} = \int_0^\infty L(\nu) \frac{G(\nu)}{G(\nu_n)} d\nu \quad \left[\lim_{\text{FWHM}/\Gamma_n \rightarrow \infty} \mathcal{L} \right] = 1 \quad \left[\lim_{\text{FWHM}/\Gamma_n \rightarrow 0} \mathcal{L} \right] = \frac{L(\nu_0)}{G(\nu_n)} = \left(\frac{\text{FWHM}}{\Gamma_n} \right) \frac{1}{\sqrt{\pi \log(2)}} \quad (22)$$

and consequently rewrite the optical pumping rate as:

$$A(r, 0) = 800 \text{ kHz} \times \left[\frac{P_0(r)}{100 \text{ W}} \right] \left[\frac{10 \text{ cm}^2}{w^2} \right] \left[\frac{\lambda_0}{894 \text{ nm}} \right] [3f_1] \left[\frac{150 \text{ GHz}}{\text{FWHM}} \right] \left[\frac{\mathcal{L}}{0.5} \right] \quad (23)$$

One last issue to consider is the N_2 non-radiative quenching rate. The spontaneous emission rate from the excited states to the ground state of Rb and Cs is about 30 MHz. The quenching rate constant due to collisions with N_2 is about 10 GHz/amg. The typical N_2 density used is at least about 0.1 amg for a quenching rate of around 1000 MHz. Because the quenching rate is much more than the spontaneous rate, the cells are not usually sensitive to radiation trapping. However stimulated emission could also result in radiation trapping if the laser power was high enough. To compare the scales, we'll note that the stimulated emission rate must be equal to the optical pumping rate. Furthermore, we'll assume a 2 inch diameter cell undergoing Cs D1 transitions:

$$\frac{\text{maximum stimulated emission}}{N_2 \text{ quenching}} \approx 10^{-3} \times \left[\frac{P_0}{100 \text{ W}} \right] \left[\frac{150 \text{ GHz}}{\text{FWHM}} \right] \left[\frac{0.1 \text{ amg}}{[N_2]} \right] \quad (24)$$

$$\frac{\text{maximum stimulated emission}}{\text{spontaneous emission}} \approx 0.03 \times \left[\frac{P_0}{100 \text{ W}} \right] \left[\frac{150 \text{ GHz}}{\text{FWHM}} \right] \quad (25)$$

Under typical conditions, $P_0 = 100 \text{ W}$, $\text{FWHM} = 750 \text{ GHz}$, $[N_2] = 0.1 \text{ amg}$: stimulated emission \ll spontaneous emission \ll N_2 quenching. Under optimal FEL conditions, $P_0 = 2000 \text{ W}$, $\text{FWHM} = 150 \text{ GHz}$, $[N_2] = 0.1 \text{ amg}$: stimulated emission \approx spontaneous emission \ll N_2 quenching. To be on the safe side, it might not be a bad idea to double the N_2 density to about 0.2 amg.

5 Laser Power Requirements

If we're willing to ignore details of the laser beam spectral profile, then we can derive some simple formulas to estimate the laser power requirements. We'll start an estimate of the change in photon flux for a *fixed* alkali polarization P_A from $z = 0$ to $z = \ell$:

$$\begin{aligned} \frac{d\Phi(\nu, r, z)}{dz} &= -[A] (1 - P_A) \sigma_1(\nu) \Phi(\nu, r, z) & (26) \\ \frac{d \int_0^\infty \Phi(\nu, r, z) d\nu}{dz} &= -[A] (1 - P_A) \int_0^\infty \sigma_1(\nu) \Phi(\nu, r, z) d\nu \\ \frac{d \int_0^\infty \phi(r, z) G(\nu) d\nu}{dz} &= -[A] \left(1 - \frac{A}{A + \Gamma'_A} \right) A \\ \frac{d\phi(r, z)}{dz} &= -[A] \left(\frac{\Gamma'_A}{A + \Gamma'_A} \right) A \\ \frac{d\phi(r, z)}{dz} &= -[A] \Gamma'_A \left(\frac{A}{A + \Gamma'_A} \right) \\ \frac{\phi(r, \ell) - \phi(r, 0)}{\ell} &\approx -[A] \Gamma'_A P_A & (27) \end{aligned}$$

where ℓ is the path length at a distance r from the center of the cell and is given by:

$$\ell(r) = 2R \sqrt{1 - \left(\frac{r}{R} \right)^2} \quad \text{spherical cell} \quad (28)$$

$$\ell(r) = 2R \quad \text{cylindrical cell} \quad (29)$$

If we integrate from $r = 0$ to the cell radius, $r = R$, we can find the total change in power:

$$\phi(r, \ell) - \phi(r, 0) = -[A] \Gamma'_A P_A \ell \quad (30)$$

$$\int_0^R 2\pi r h \nu_0 (\phi(r, \ell) - \phi(r, 0)) dr = -h \nu_0 [A] \Gamma'_A P_A \int_0^R 2\pi r \ell dr \quad (31)$$

Note that for either type of cell, the radial integral over $\ell(r)$ simply results in the volume of the pumping chamber:

$$\int_0^R 2\pi r \ell dr = V_{pc} \quad (32)$$

The change in power is negative because the alkali atoms in the cell are absorbing the light and transforming it into heat:

$$\Delta P_0 \approx -h\nu_0[A]\Gamma'_A P_A V_{pc} = -140 \text{ W} \times \left[\frac{P_A}{0.9} \right] \left[\frac{894 \text{ nm}}{\lambda_0} \right] \left[\frac{[A]}{10^{14}/\text{cm}^3} \right] \left[\frac{\Gamma'_A}{100 \text{ kHz}} \right] \left[\frac{V_{pc}}{70 \text{ cc}} \right] \quad (33)$$

To figure out the minimum amount of laser power at the *front* of the cell to maintain a fixed alkali polarization P_A *throughout* the cell, we'll first need to consider the minimum photon flux needed to maintain P_A at the *back* of the cell, $z = \ell$:

$$\begin{aligned} P_A &= \frac{A}{A + \Gamma'_A} & (34) \\ A &= \Gamma'_A \frac{P_A}{1 - P_A} \\ \int_0^\infty \Phi(\nu, r, \ell) \sigma_1(\nu) d\nu &= \Gamma'_A \left[\frac{P_A}{1 - P_A} \right] \\ \phi(r, \ell) \pi f_1 r_e c \int_0^\infty G(\nu) L(\nu) d\nu &= \Gamma'_A \left[\frac{P_A}{1 - P_A} \right] \\ \phi(r, \ell) \pi f_1 r_e c G(\nu_0) \mathcal{L} &= \Gamma'_A \left[\frac{P_A}{1 - P_A} \right] \\ \phi(r, \ell) &= \left[\frac{\Gamma'_A}{\pi f_1 r_e c G(\nu_0) \mathcal{L}} \right] \left[\frac{P_A}{1 - P_A} \right] & (35) \end{aligned}$$

The minimum photon flux needed at the front of the cell $z = 0$ is the previous quantity plus the amount of flux absorbed over the full path length:

$$\phi(r, 0) = \underbrace{[A]\Gamma'_A P_A \ell(r)}_{\Delta\phi} + \underbrace{\left[\frac{\Gamma'_A}{\pi f_1 r_e c G(\nu_0) \mathcal{L}} \right] \left[\frac{P_A}{1 - P_A} \right]}_{\phi(r, \ell)} \quad (36)$$

For a spherical cell, the highest incident photon flux and longest path length occur at the center of the cell ($r = 0, \ell = 2R$), whereas the lowest flux and shortest path length occur at the edge of the cell ($r = R, \ell = 0$). Therefore, we'll calculate the total minimum power of the beam needed to maintain an alkali polarization of P_A by evaluating the previous equation at both $r = 0$ and $r = R$.

At the edge of the cell, we find:

$$\phi(R, 0) = \left[\frac{\Gamma'_A}{\pi f_1 r_e c G(\nu_0) \mathcal{L}} \right] \left[\frac{P_A}{1 - P_A} \right] \quad (37)$$

$$\frac{P_0}{h\nu_0} \frac{2}{w^2 \pi} \exp\left(-\frac{2R^2}{w^2}\right) = \left[\frac{\Gamma'_A}{\pi f_1 r_e c G(\nu_0) \mathcal{L}} \right] \left[\frac{P_A}{1 - P_A} \right] \quad (38)$$

$$P_0 = \underbrace{\left[w^2 \exp\left(+\frac{2R^2}{w^2}\right) \right]}_f \left[\frac{h\Gamma'_A}{2f_1 r_e \lambda_0 G(\nu_0) \mathcal{L}} \right] \left[\frac{P_A}{1 - P_A} \right] \quad (39)$$

Before going further, it's useful to find the value for the beam radius w that minimizes f :

$$\frac{\partial f}{\partial w^2} = w^2 \left(\frac{-2R^2}{w^4} \right) \exp\left(\frac{2R^2}{w^2}\right) + \exp\left(\frac{2R^2}{w^2}\right) = \frac{f}{w^2} \left(1 - \frac{2R^2}{w^2} \right) = 0 \rightarrow w = R\sqrt{2} \quad (40)$$

Using the minimum intensity at the edge of the cell as a constraint, we find the minimum total beam power:

$$P_0 = 308 \text{ W} \times \left[\frac{w^2}{10 \text{ cm}^2} \right] \exp\left(\frac{2R^2}{w^2} - 1\right) \left[\frac{\Gamma'_A}{100 \text{ kHz}} \right] \frac{1}{3f_1} \left[\frac{894 \text{ nm}}{\lambda_0} \right] \left[\frac{\text{FWHM}}{150 \text{ GHz}} \right] \left[\frac{0.5}{\mathcal{L}} \right] \left[\frac{0.1P_A}{0.9(1 - P_A)} \right] \quad (41)$$

Using the minimum intensity at the back of the cell plus the power absorbed through the center of the cell as a constraint, we find an alternative minimum total beam power:

$$\phi(0,0) = [A]\Gamma'_A P_A(2R) + \left[\frac{\Gamma'_A}{\pi f_1 r_e c G(\nu_0) \mathcal{L}} \right] \left[\frac{P_A}{1 - P_A} \right] \quad (42)$$

$$\begin{aligned} \frac{2P_0}{h\nu_0 \pi w^2} &= [A]\Gamma'_A P_A(2R) + \left[\frac{\Gamma'_A}{\pi f_1 r_e c G(\nu_0) \mathcal{L}} \right] \left[\frac{P_A}{1 - P_A} \right] \\ P_0 &= 157 \text{ W} \left[\frac{w^2}{10 \text{ cm}^2} \right] \left[\frac{894 \text{ nm}}{\lambda_0} \right] \left[\frac{\Gamma'_A}{100 \text{ kHz}} \right] \left[\frac{P_A}{0.9} \right] \left[\frac{[A]}{10^{14}/\text{cm}^3} \right] \left[\frac{2R}{5 \text{ cm}} \right] \\ &+ 113 \text{ W} \left[\frac{w^2}{10 \text{ cm}^2} \right] \left[\frac{894 \text{ nm}}{\lambda_0} \right] \left[\frac{\Gamma'_A}{100 \text{ kHz}} \right] \left[\frac{0.1P_A}{0.9(1 - P_A)} \right] \left[\frac{1}{3f_1} \right] \left[\frac{\text{FWHM}}{150 \text{ GHz}} \right] \left[\frac{0.5}{\mathcal{L}} \right] \end{aligned} \quad (43)$$

These two estimates for the total laser power required are constrained by the fact that the beam spatial profile can only be controlled to a certain degree. It would be ideal to shape the beam to match the path length profile of the cell, but that is not always possible. Therefore some of the laser power is necessarily thrown away or used inefficiently.

6 Discussion

It's useful to re-express the previous equations in terms of Xe quantities. Because we are working with amagats of Xe, we can make the following substitutions:

1. We'll express the alkali density as the desired alkali to Xe-129 polarization ratio and the Xe wall relaxation rate:

$$[\text{Cs}] = \left(\frac{\Gamma_{\text{wall}}}{k_{\text{se}}} \right) \left(\frac{P_{129}}{P_{\text{Cs}}} \right) \left(1 - \frac{P_{129}}{P_{\text{Cs}}} \right)^{-1} \quad (44)$$

$$k_{\text{se}} = \langle \sigma v \rangle_2 \left(1 + \frac{[\text{Xe}]_3}{[\text{Xe}]} \right) \approx \langle \sigma v \rangle_2 \times 1.1 \quad (45)$$

2. We'll express the alkali relaxation rate as the Xe density, since collisions with Xe is the dominant source of alkali relaxation.

$$\Gamma'_{\text{Cs}} \approx [\text{Xe}]k_{\text{sd}} \left(1 + 0.5 \times \frac{[129]k_{\text{se}}}{[\text{Xe}]k_{\text{sd}}} + \frac{[131]k'_{\text{se}}}{[\text{Xe}]k_{\text{sd}}} \right) \approx [\text{Xe}]k_{\text{sd}} \times 1.3 \quad (46)$$

3. We'll express the pressure broadened linewidth as the Xe density, since the Xe density is much more than the N₂ density.

$$\Gamma_1 = (19 \text{ GHz/amg}) ([\text{Xe}] + [\text{N}_2]) \approx (20 \text{ GHz/amg}) [\text{Xe}] \quad (47)$$

Using these substitutions, we get the following for the total power absorbed:

$$\Delta P_0 \approx -3.3 \text{ W} \times \left[\frac{P_{129}}{0.5} \right] \left[\frac{0.4}{1 - P_{129}/P_{\text{Cs}}} \right] \left[\frac{300 \text{ sec}}{\Gamma_{\text{wall}}^{-1}} \right] \left[\frac{[\text{Xe}]}{1 \text{ amg}} \right] \left[\frac{V_{\text{pc}}}{70 \text{ cc}} \right] \quad (48)$$

The minimum total power estimated from using the edge intensity as a constraint is:

$$P_0 = 65 \text{ W} \times \left[\frac{[\text{Xe}]}{1 \text{ amg}} \right] \left[\frac{\text{FWHM}}{150 \text{ GHz}} \right] \left[\frac{0.5}{\mathcal{L}} \right] \left[\frac{0.1P_A}{0.9(1 - P_A)} \right] \left[\frac{w^2}{10 \text{ cm}^2} \right] \exp \left(\frac{2R^2}{w^2} - 1 \right) \quad (49)$$

The minimum total power estimated using the center intensity as a constraint is:

$$\begin{aligned} P_0 &= 3.8 \text{ W} \left[\frac{[\text{Xe}]}{1 \text{ amg}} \right] \left[\frac{P_{129}}{0.5} \right] \left[\frac{0.4}{1 - P_{129}/P_{\text{Cs}}} \right] \left[\frac{300 \text{ sec}}{\Gamma_{\text{wall}}^{-1}} \right] \left[\frac{2R}{5 \text{ cm}} \right] \left[\frac{w^2}{10 \text{ cm}^2} \right] \\ &+ 24 \text{ W} \left[\frac{[\text{Xe}]}{1 \text{ amg}} \right] \left[\frac{0.1P_A}{0.9(1 - P_A)} \right] \left[\frac{\text{FWHM}}{150 \text{ GHz}} \right] \left[\frac{0.5}{\mathcal{L}} \right] \left[\frac{w^2}{10 \text{ cm}^2} \right] \end{aligned} \quad (50)$$

7 Notes on SEOP Simulation

The equations derived in the previous sections ignore the details of the laser beam spectral profile. Whereas those equations correctly count the number of photons removed from the beam, they do not keep track of what frequencies those lost photons are. They assume that the spectral profile remains a gaussian *throughout* the cell. In real life, the spectral profile of the beam develops a “hole” corresponding to the absorption peak of the alkali atoms. A full simulation is needed to account for the fact that the laser beam spectral profiles do not remain gaussian as it propagates through the cell. If I were to do the full Cs-Xe SEOP simulation, then, for the record, I would use the following equations, taking into account the assumptions listed in the previous sections:

$$P_{\text{Cs}}(r, z) = \frac{A(r, z)}{A(r, z) + \Gamma'_{\text{Cs}}} \quad (51)$$

$$P_{129}(r, z) = P_{\text{Cs}}(r, z) \left[\frac{k_{\text{se}}[\text{Cs}]}{k_{\text{se}}[\text{Cs}] + \Gamma_{129}} \right] \quad (52)$$

$$P_{131}(r, z) = P_{\text{Cs}}(r, z) \left[\frac{k'_{\text{se}}[\text{Cs}]}{k'_{\text{se}}[\text{Cs}] + \Gamma_{131}} \right] \quad (53)$$

where the relaxation rates are given by the rate constants in table blah and these equations:

$$\Gamma'_{\text{Cs}} = k_{\text{sd}}[\text{Xe}] + \left(\frac{k_{\text{se}}[129]}{k_{\text{se}}[\text{A}] + \Gamma_{129}} \right) \Gamma_{129} + \left(\frac{k'_{\text{se}}[131]}{k'_{\text{se}}[\text{A}] + \Gamma_{131}} \right) \Gamma_{131} + k'_{\text{sd}}[\text{Cs}] + k''_{\text{sd}}[\text{N}_2] \quad (54)$$

$$\Gamma_{129} = \Gamma_{\text{wall}} \quad (55)$$

$$\Gamma_{131} = \Gamma_{\text{wall}} + k''_{\text{sd}}[\text{Xe}] \quad (56)$$

As mentioned before, we're using isotopically enriched Xe:

$$[\text{Xe}] = 0.8 \times [129] + 0.2 \times [131] \quad (57)$$

and the number density of Cs is given by the following formula adapted from the 1995 CRC:

$$[\text{Cs}] = 10^{14}/\text{cm}^3 \times \left(\frac{400 \text{ K}}{T} \right) \exp \left[21.71 - 22.05 \left(\frac{400 \text{ K}}{T} \right) \right] \quad (58)$$

The optical pumping rate would be a numerical integration of the following:

$$A(r, z) = \pi f_1 r_e c \int_0^\infty \Phi(\nu, r, z) L(\nu) d\nu \quad (59)$$

The D1 oscillator strength for Cs is $f_1 = 0.37$, which is an average of the NIST & Radzig value. We'll use a simple symmetric lorentzian for the absorption lineshape and estimate the pressure broadened width using the Rb numbers:

$$L(\nu) = \frac{\Gamma_1/2\pi}{(\nu - \nu_1)^2 + \Gamma_1^2/4} \quad (60)$$

$$\Gamma_1 = (19 \text{ GHz/amg}) ([\text{Xe}] + [\text{N}_2]) \quad (61)$$

where the initial photon flux would be given by a gaussian spectrum and gaussian beam profile:

$$\Phi(\nu, r, 0) = 1.8 \times 10^8/\text{cm}^2 \times \left[\frac{P_0}{100 \text{ W}} \right] \left[\frac{10 \text{ cm}^2}{w^2} \right] \left[\frac{\lambda_0}{894 \text{ nm}} \right] \left[\frac{150 \text{ GHz}}{\text{FWHM}} \right] \exp \left(-\frac{2r^2}{w^2} - \left[\frac{5(\nu - \nu_0)}{3 \cdot \text{FWHM}} \right]^2 \right) \quad (62)$$

The photon flux of the propagating beam would be determined by:

1. Calculating the optical pumping rate at z
2. Calculating the polarizations at z
3. Calculating the photon flux at $z + \Delta z$ using

$$\Phi(\nu, r, z + \Delta z) = \Phi(\nu, r, z) \exp(-\pi f_1 r_e c [\text{Cs}] (1 - P_{\text{Cs}}(r, z)) L(\nu) \Delta z) \quad (63)$$