

Basics of rubidium-xenon spin-exchange optical pumping

Magnetising xenon gas

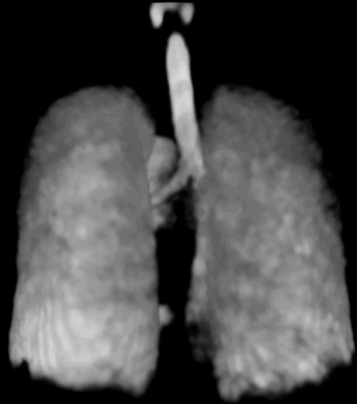
Graham Norquay

Aarhus MR workshop Oct 2026

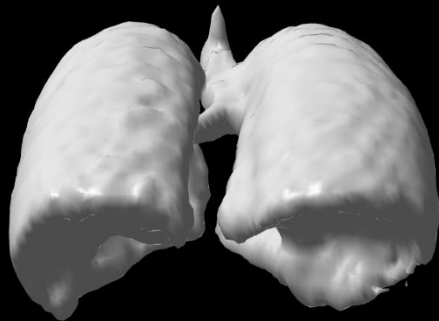
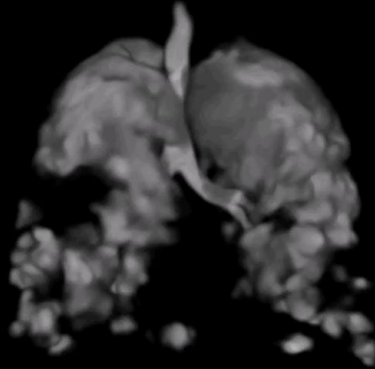
g.norquay@sheffield.ac.uk

Hyperpolarised ^{129}Xe MRI

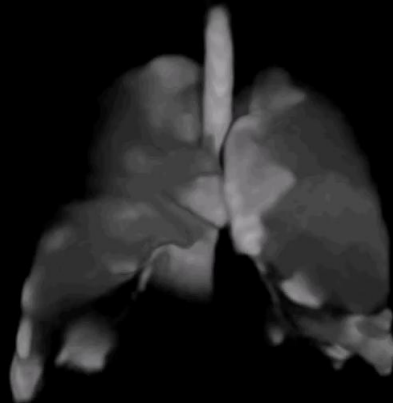
Healthy



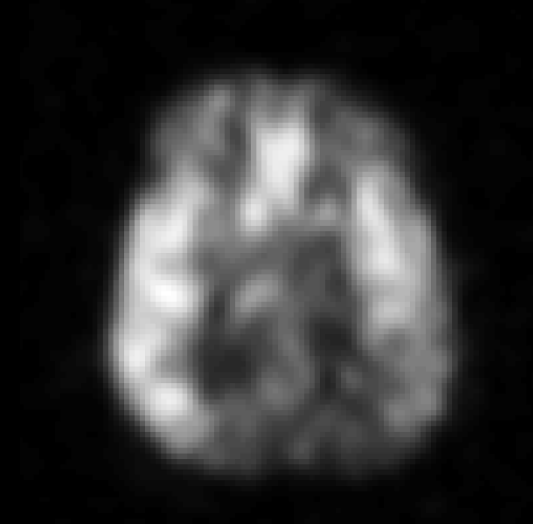
COPD



Gas-phase ^{129}Xe

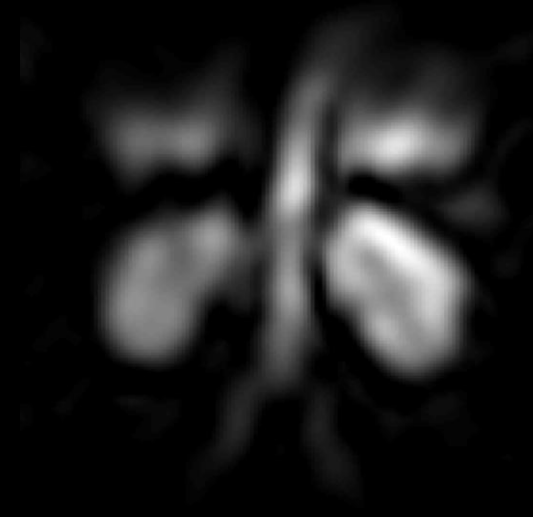


Dissolved-phase ^{129}Xe



Human brain

Rao et al,
Radiology, 286,
2018



Human kidneys

Chacon-Caldera
et al., MRM(83)
2019

OPTICAL PUMPING

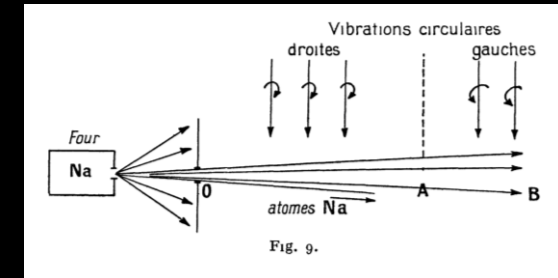
Optical pumping



Alfred Kastler

Awarded 1966 Nobel prize in physics “for the discovery and development of optical methods for studying Hertzian resonances in atoms”

A. Kastler. “Some suggestions concerning the production and detection by optical means of inequalities in the populations of levels of spatial quantization in atoms. Application to the Stern and Gerlach and magnetic resonance experiments. *J. Phys. Radium*, **11**, 255. (1950)



“The use of circularly polarised light creates an asymmetry of population between negative m levels and positive m levels, the direction of this asymmetry being able to be reversed by reversing the direction of circular polarisation of the incident light”

Optical pumping with alkali metals

- λ in visible and near-IR (590-865 nm) – relatively inexpensive, high-power lasers available
- High volatility – dense vapours at relatively low temperatures [MP = 27°C (Fr) to 181°C (Li)]
- Single valence electron in *s* subshell – efficient optical pumping and straightforward transition analysis

	Li	Na	K	Rb	Cs	Fr
Z	3	11	19	37	55	87
Configuration	[He]2s	[Ne]3s	[Ar]4s	[Kr]5s	[Xe]6s	[Rn]7s
IP (eV)	5.3917	5.1391	4.3407	4.1771	3.8939	4.073
$\lambda(S-P_{1/2})$ (Å)	6709.77	5897.56	7701.08	7949.78	8945.93	8171.66
$\lambda(S-P_{3/2})$ (Å)	6709.62	5891.58	7667.01	7802.41	8523.47	7181.85
ΔE_{FS} (cm ⁻¹)	0.34	17.20	57.71	237.60	554.04	1687
$\tau(nP_{1/2})$ (ns)	27.10 [8]	16.28 [9]	26.69 [10]	27.75 [11]	34.88 [12]	29.45 [13]
$f_{1/2}$	0.249	0.320	0.333	0.341	0.344	0.339
$\tau(nP_{3/2})$ (ns)	27.10 [8]	16.23 [9]	26.34 [10]	26.25 [11]	30.462 [12]	21.0 [14]
$f_{3/2}$	0.497	0.641	0.669	0.695	0.715	0.734
μ_{ns}	0.399 – 0.061 <i>E</i>	1.348 – 0.132 <i>E</i>	2.180 – 0.314 <i>E</i>	3.130 – 0.419 <i>E</i>	4.048 – 0.573 <i>E</i>	5.07 – 0.556 <i>E</i>
μ_{np}	0.047 + 0.050 <i>E</i>	0.854 – 0.258 <i>E</i>	1.711 – 0.542 <i>E</i>	2.645 – 0.681 <i>E</i>	3.568 – 0.889 <i>E</i>	
μ_{nd}	0.002 + 0.009 <i>E</i>	0.015 + 0.081 <i>E</i>	0.278 + 2.137 <i>E</i>	1.353 + 1.760 <i>E</i>	2.476 + 0.372 <i>E</i>	3.41 – 0.095 <i>E</i>

Alkali metal atoms

(assuming zero nuclear spin)

Group → 1

↓ Period

1	1 H
2	3 Li
3	11 Na
4	19 K
5	37 Rb
6	55 Cs
7	87 Fr

Orange Na Doublet:

Near-IR Rb Doublet:

$\lambda_{D2} = 780.0 \text{ nm}$

D_2

D_1

$\lambda_{D1} = 794.8 \text{ nm}$

$\text{Rb} = [\text{Kr}]5s^1$

Notation:

$n \ 2S+1 L_J$

$5^2P_{3/2}$

$5^2P_{1/2}$

$5^2S_{1/2}$

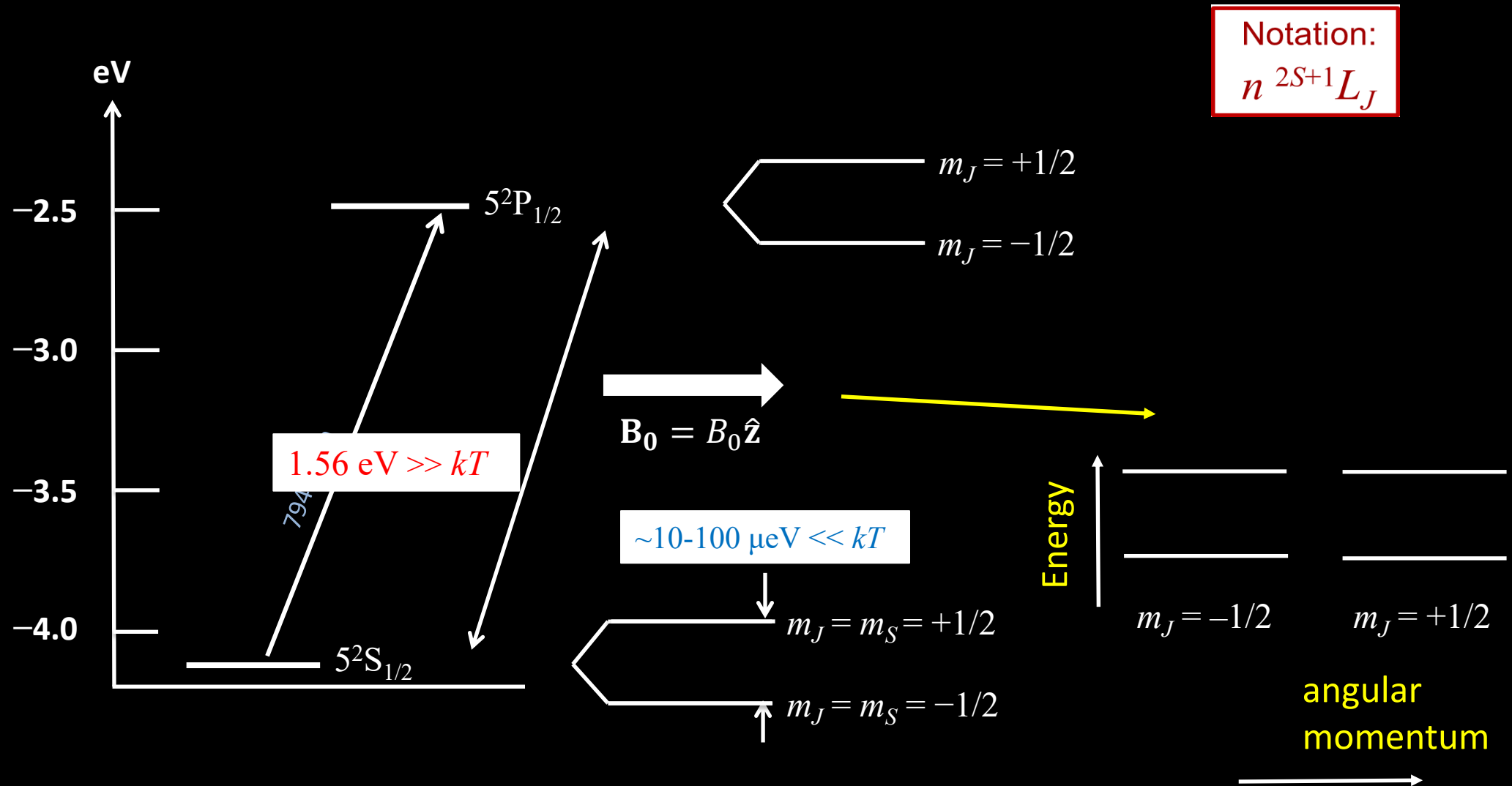
Selection rules for
electric dipole transitions:

$$\Delta L = \pm 1$$

$$\Delta J = 0, \pm 1$$

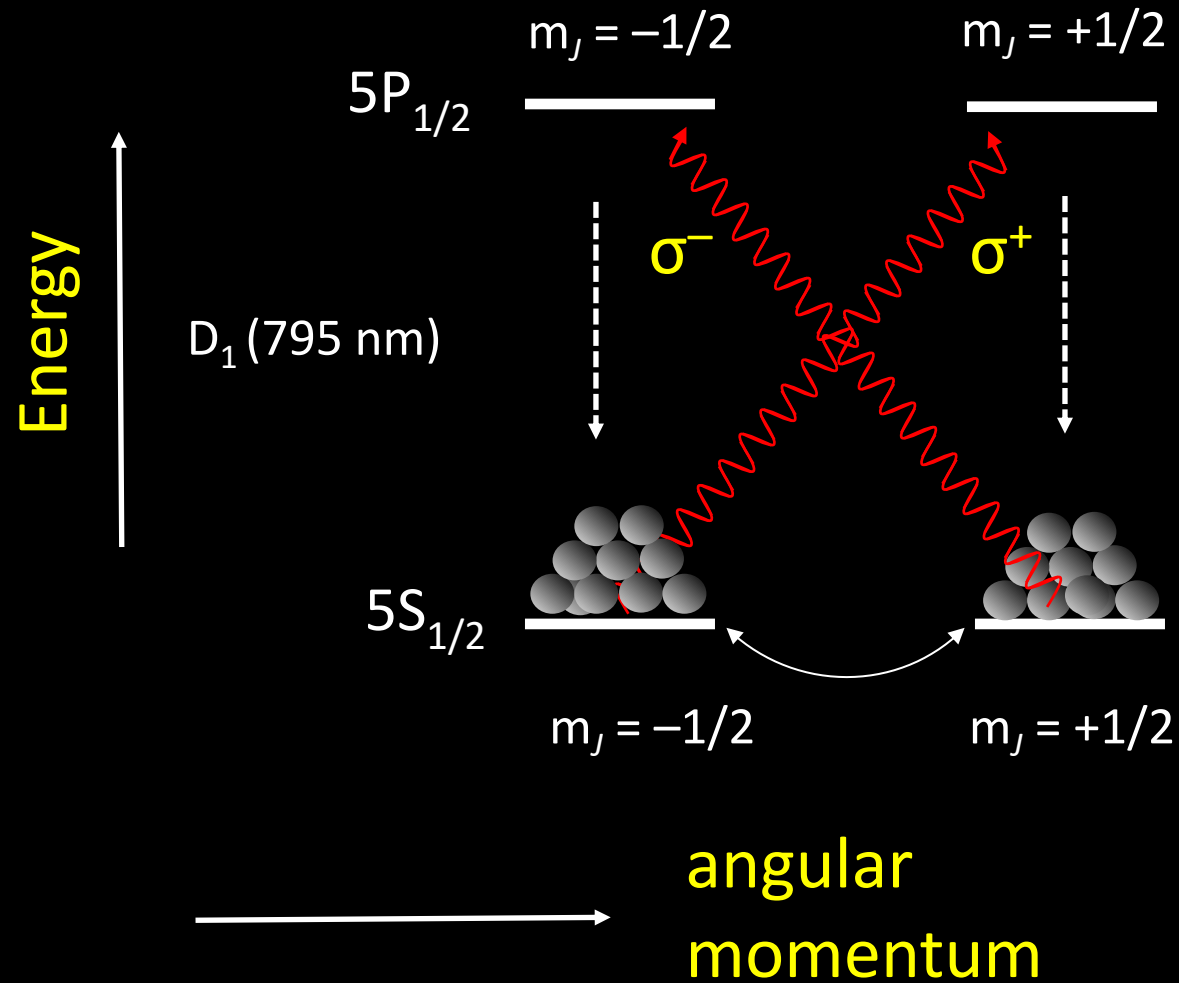
D₁ transition & Zeeman splitting in Rb

(assuming zero nuclear spin)

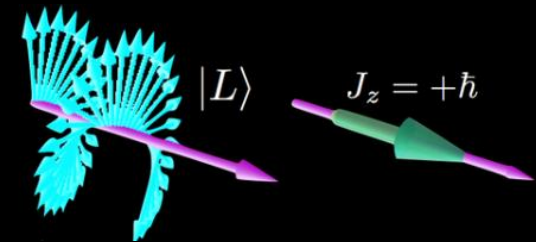


Optical pumping with rubidium

(still assuming zero nuclear spin)



Left-circularly polarised light
parallel to B_z σ^+



Additional selection rule for OP :

$$\Delta m_j = +1$$

Each polarised ground state
represents a 'dark state'

$$\sigma^- \longrightarrow m_j = -1/2$$

$$\sigma^+ \longrightarrow m_j = +1/2$$

More realistic energy-level diagram

(all alkali metals have non-zero nuclear spin)

^{87}Rb

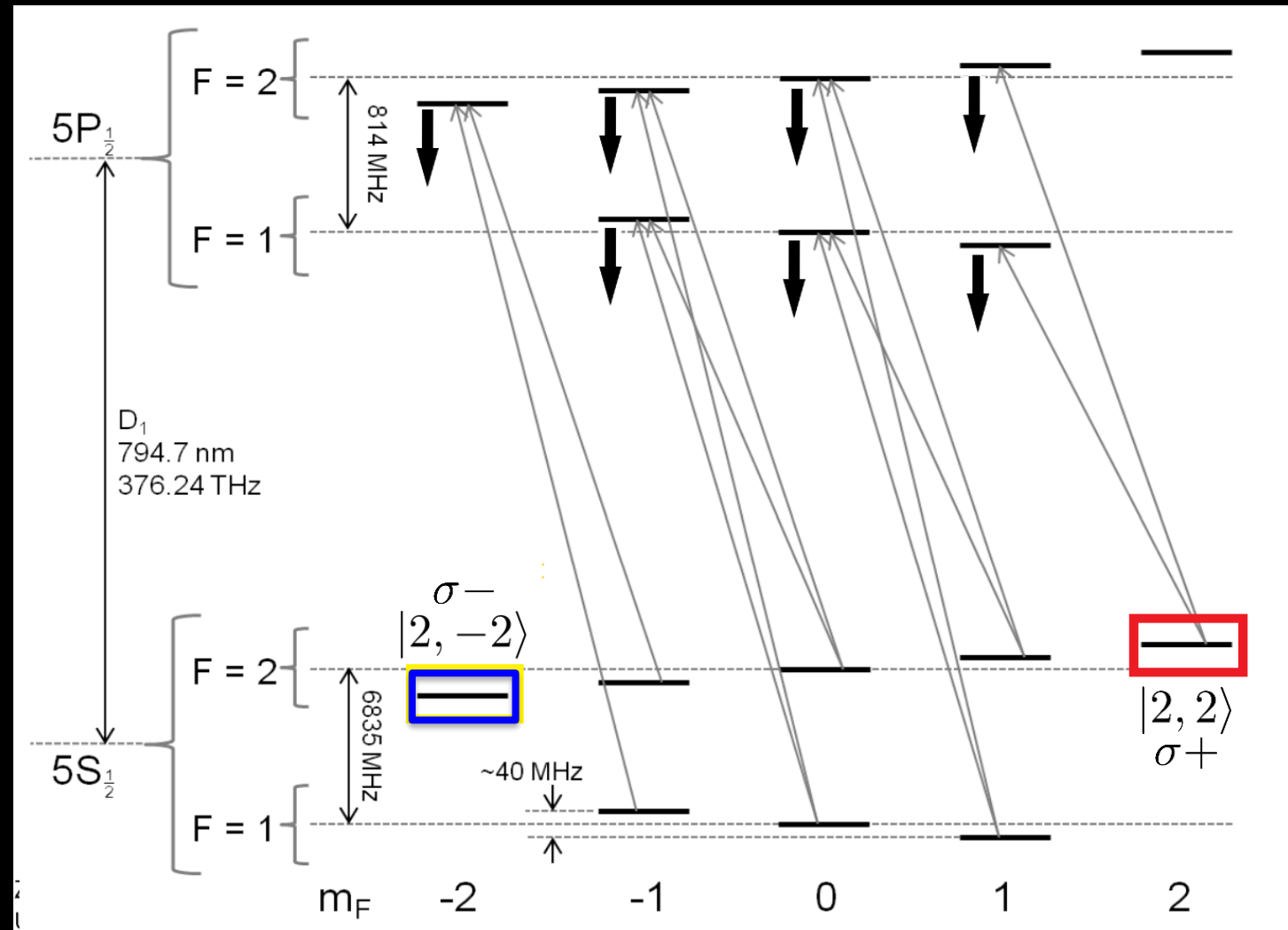
nuclear spin
 $I = 3/2$

Transition arrows to
left ($\Delta m_F = -1$) for
 σ^- light

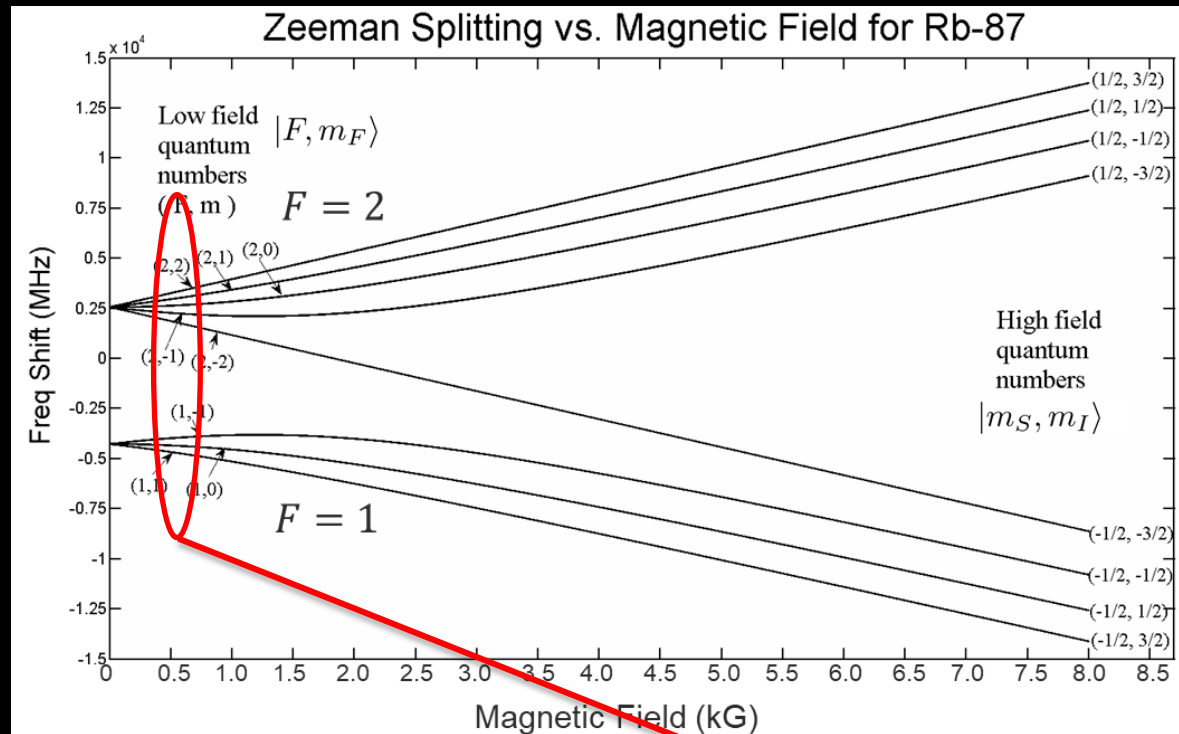
Dark states:

$\sigma^- \longrightarrow |2, -2\rangle$

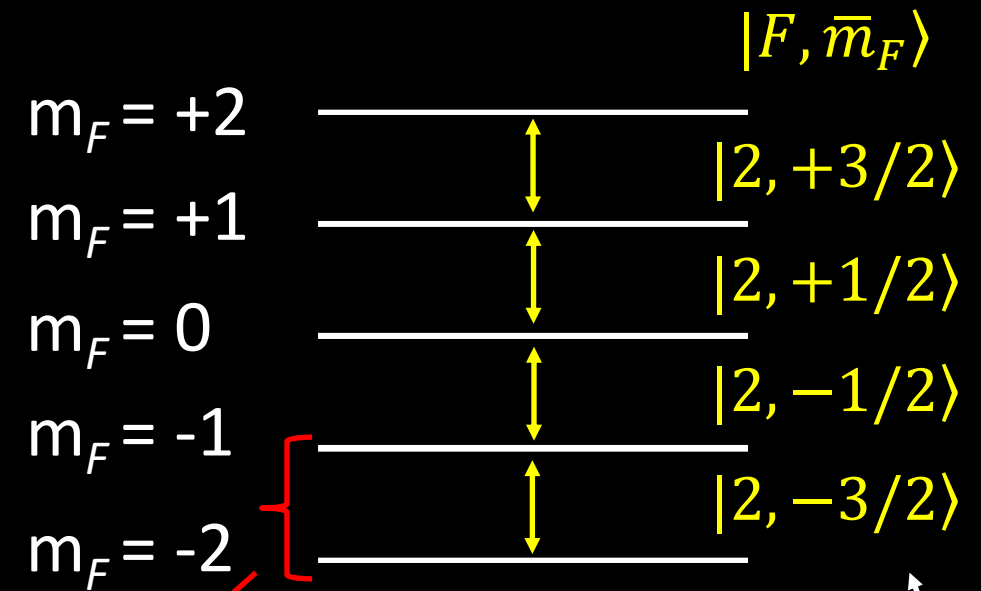
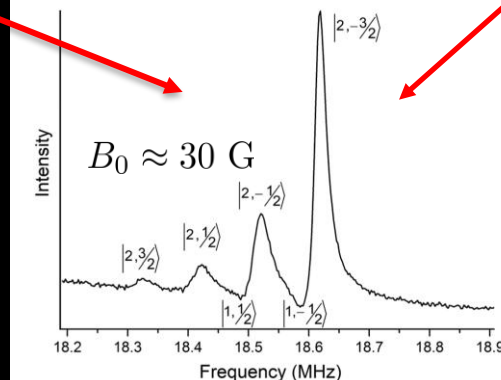
$\sigma^+ \longrightarrow |2, +2\rangle$



Rb polarimetry from ground-state hyperfine structure



Ground-state hyperfine spectrum generated by optically detected EPR (ODEPR)



$$\bar{m}_F = \frac{-2 + (-1)}{2} = -\frac{3}{2}$$

Ratio of peak intensities $\rightarrow P_A$

Electronic Rb polarisation

SPIN-EXCHANGE

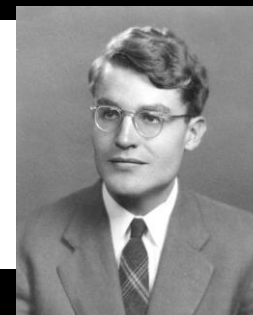
First SEOP Paper (1960)*



Marie-Ann Bouchiat

NUCLEAR POLARIZATION IN He^3 GAS INDUCED BY OPTICAL PUMPING AND DIPOLAR EXCHANGE*

M. A. Bouchiat,[†] T. R. Carver,[‡] and C. M. Varnum
Palmer Physical Laboratory, Princeton University, Princeton, New Jersey
(Received September 26, 1960)

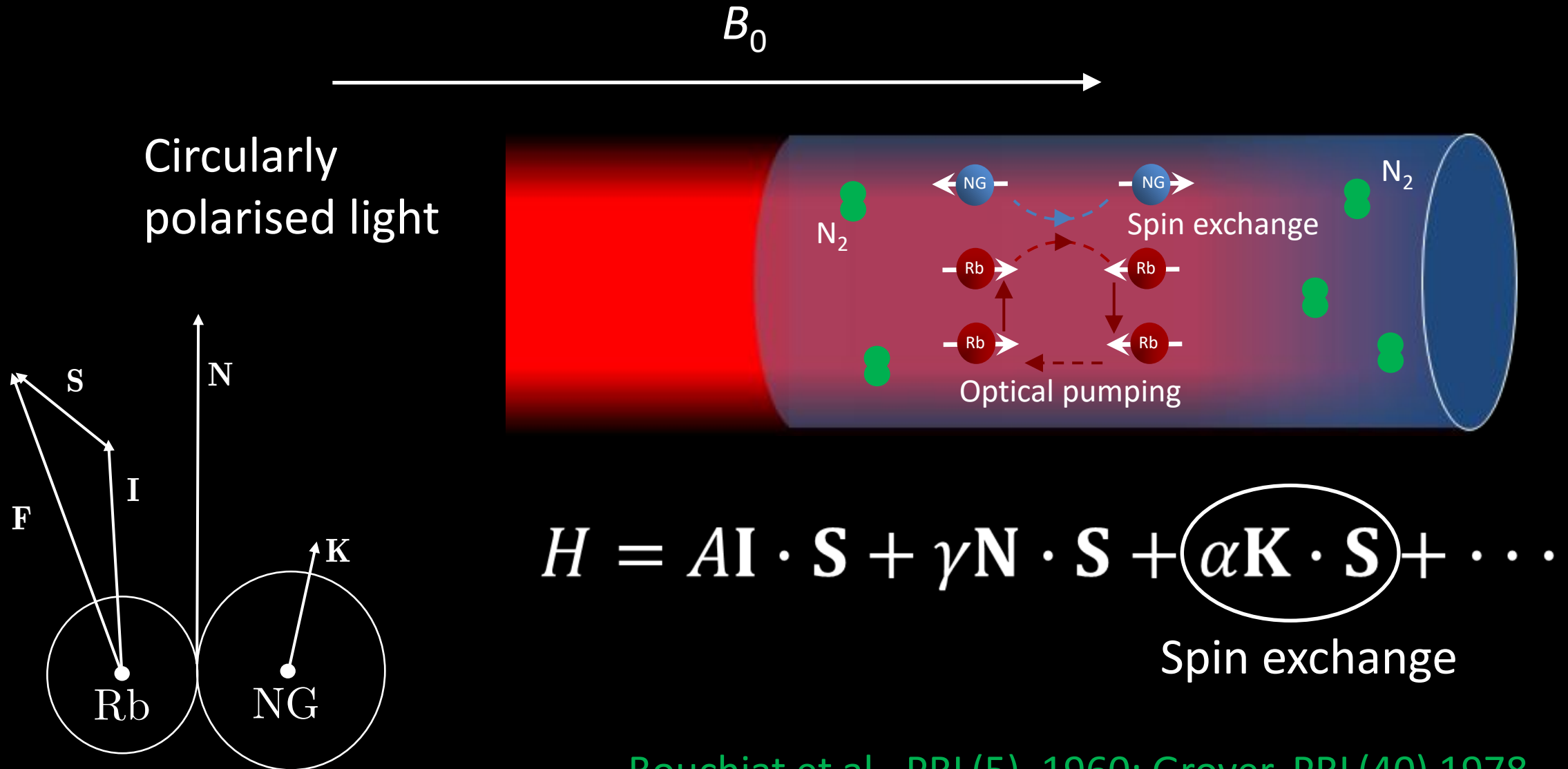


Tom Carver

“...the Overhauser effect should work not by the dipole-coupled relaxation of a saturated paramagnetic impurity toward a polarized equilibrium, but by the relaxation of an optically polarized impurity toward a nearly depolarized equilibrium.”

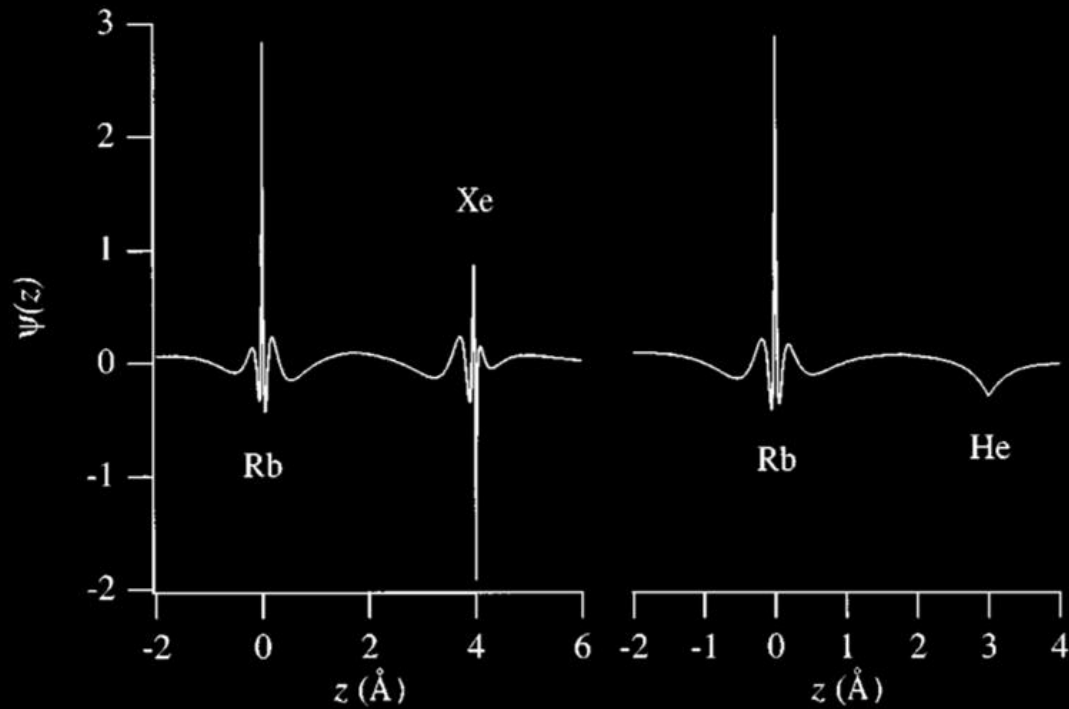
*M.A. Bouchiat, T.R. Carver, and C.M. Varnum, *Phys. Rev. Lett.* **5**, 373

Mixing polarised rubidium vapour with noble gases: SEOP



Bouchiat et al., PRL(5), 1960; Grover, PRL(40) 1978

Binary spin exchange: Xe vs He



Greater Rb electron overlap at Xe nucleus → stronger spin-exchange

Walker&Happer RMP(69), 1997

$$\gamma_{se} = [\text{Rb}] \gamma' \approx 10^{14} \times \begin{cases} 6.8 \times 10^{-20} \text{ cm}^3/\text{s} \\ 2.2 \times 10^{-16} \text{ cm}^3/\text{s} \end{cases}$$

$$\text{Binary spin-exchange rate:} \approx \begin{cases} (40 \text{ hr})^{-1} & \text{He} \\ (50 \text{ sec})^{-1} & \text{Xe} \end{cases}$$

He

Xe

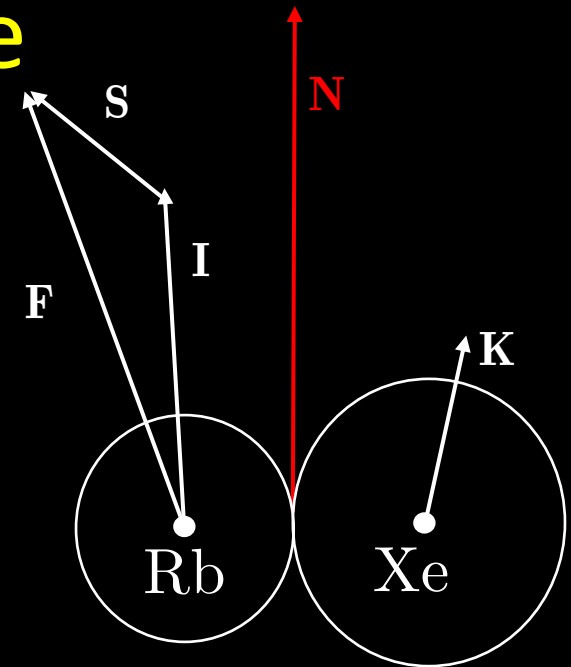
3000 times faster
for Xe!

^{129}Xe readily destroys Rb electronic polarisation

$$\Gamma_{\text{Rb}}(1 \text{ amagat}) = \begin{cases} 2.4 \times 10^5 / \text{s} & \text{Xe} \\ 45 / \text{s} & \text{He} \end{cases}$$

$$H = A\mathbf{I} \cdot \mathbf{S} + \gamma\mathbf{N} \cdot \mathbf{S} + \alpha\mathbf{K} \cdot \mathbf{S} + \dots$$

Spin-rotation interaction at xenon core



Challenge: need to use lean mixtures of Xe or low Rb vapour densities

Two methods to polarise ^{129}Xe with spin-exchange optical pumping

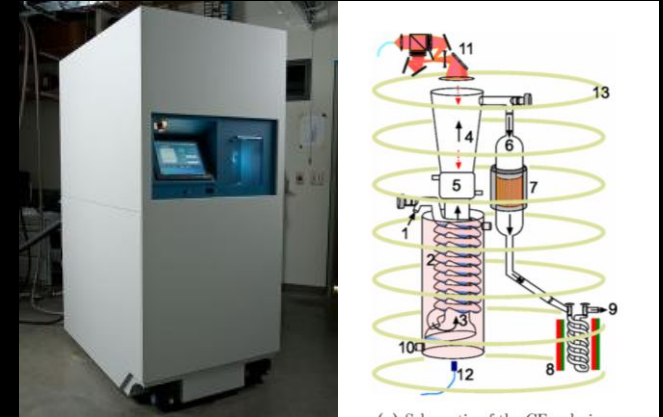
Continuous-flow: ^{129}Xe polarised with cryogenic Xe accumulation



Sheffield SpinTec Ltd



Polarean 9820



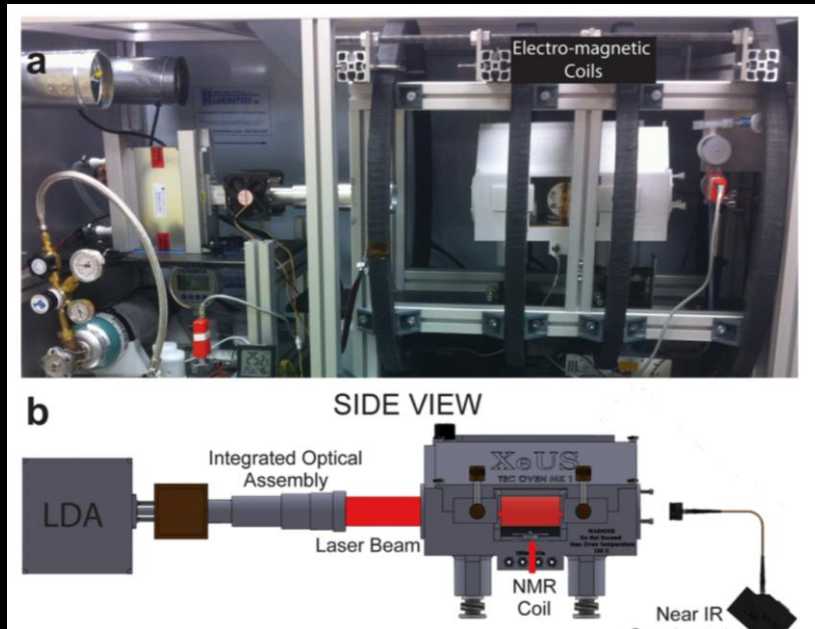
Xemed, XeBox-E10, [Ruset et al., PRL\(96\), 2006](#)

Other continuous-flow polarisers

[Driehuys et al, APL\(69\), 1996](#); [Haake et al., JACS\(119\), 1997](#); [Rosen et al., RSI\(70\), 1999](#); [Zook et al., JMR\(159\), 2002](#); [Mortuza et al., JCP\(118\), 2003](#); [Knagge et al., CPL\(397\), 2004](#); [Schrank et al., PRA\(80\), 2009](#); [Norquay et al., JAP\(113\), 2013](#). [Korchak et al., AMR\(44\), 2013](#); [Norquay et al., Phys Rev Lett\(121\), 2018](#).

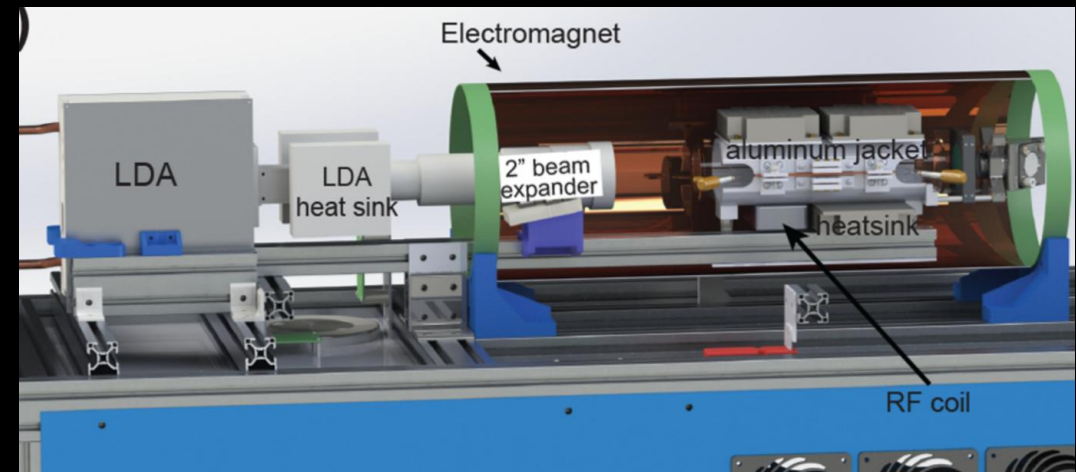
Two methods to polarise ^{129}Xe with spin-exchange optical pumping

Stopped-flow: ^{129}Xe polarised without cryogenic Xe accumulation



Nikolaou et al., JPC(118), 2014.

Other stopped-flow polarisers



Birchall et al., AC(92), 2020.

Birchall et al., Molecules(27), 2022; Raftery et al., PRL(66), 1991; Whiting et al., JMR(208), 2011; Six et al., PloS one(7), 2012; Hughes-Riley et al., JMR(237), 2013; Nikolaou et al., AC(86), 2014; Birchall et al., JMR(315), 2020.

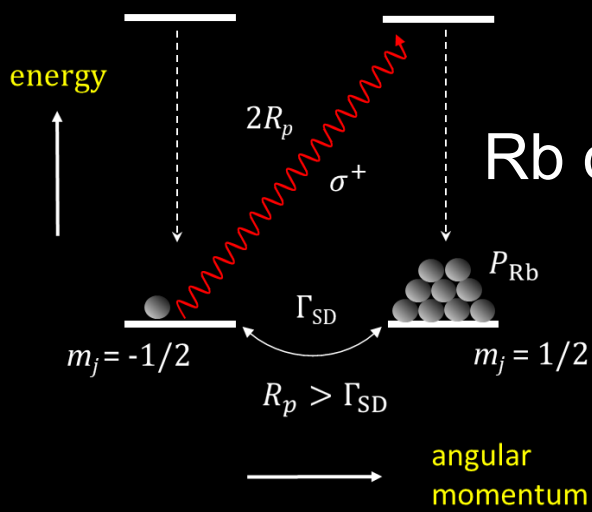
Stopped-flow vs continuous-flow

	Stopped-flow	Continuous-flow
Cryogenic separation of Xe	No	Yes
Xe in gas mix	>10%	1–3%
Laser powers	50–170 W	50–170 W
Typical ^{129}Xe polarisation	30%–95%	10%–50%
Xe production rates	100s ml/h	1000s ml/h
Low cell temp	$[\text{Rb}] \leq 10^{12} \text{ cm}^{-3}$	$[\text{Rb}] 10^{12} - 10^{14} \text{ cm}^{-3}$

Stopped-flow: Higher ^{129}Xe polarisations, lower Xe production rates

Continuous-flow: Lower ^{129}Xe polarisations, higher Xe production rates

Continuous-flow ^{129}Xe -Rb SEOP



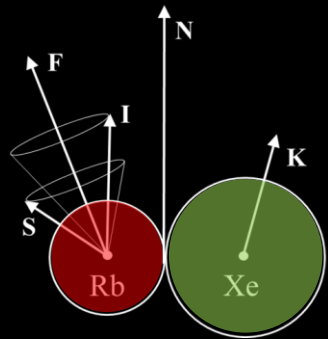
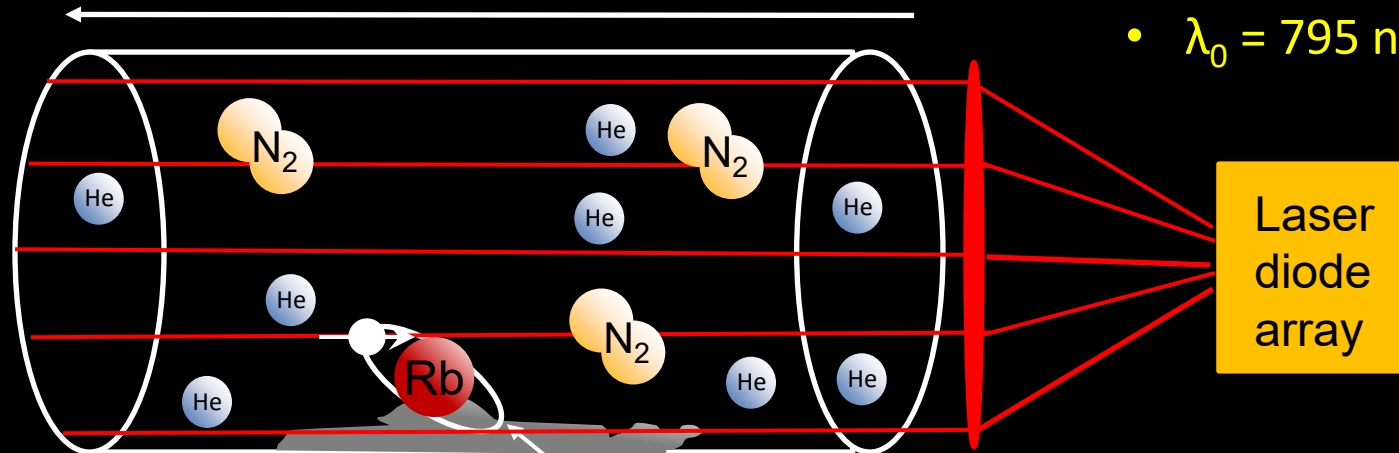
Rb optical pumping

1–3% Xe

Need to purify – cryogenic separation...

$B_0 = 10\text{--}50\text{ G}$

- Circularly polarised light
- σ^+ helicity
- $\lambda_0 = 795\text{ nm}$



Incoming xenon

Bed of rubidium

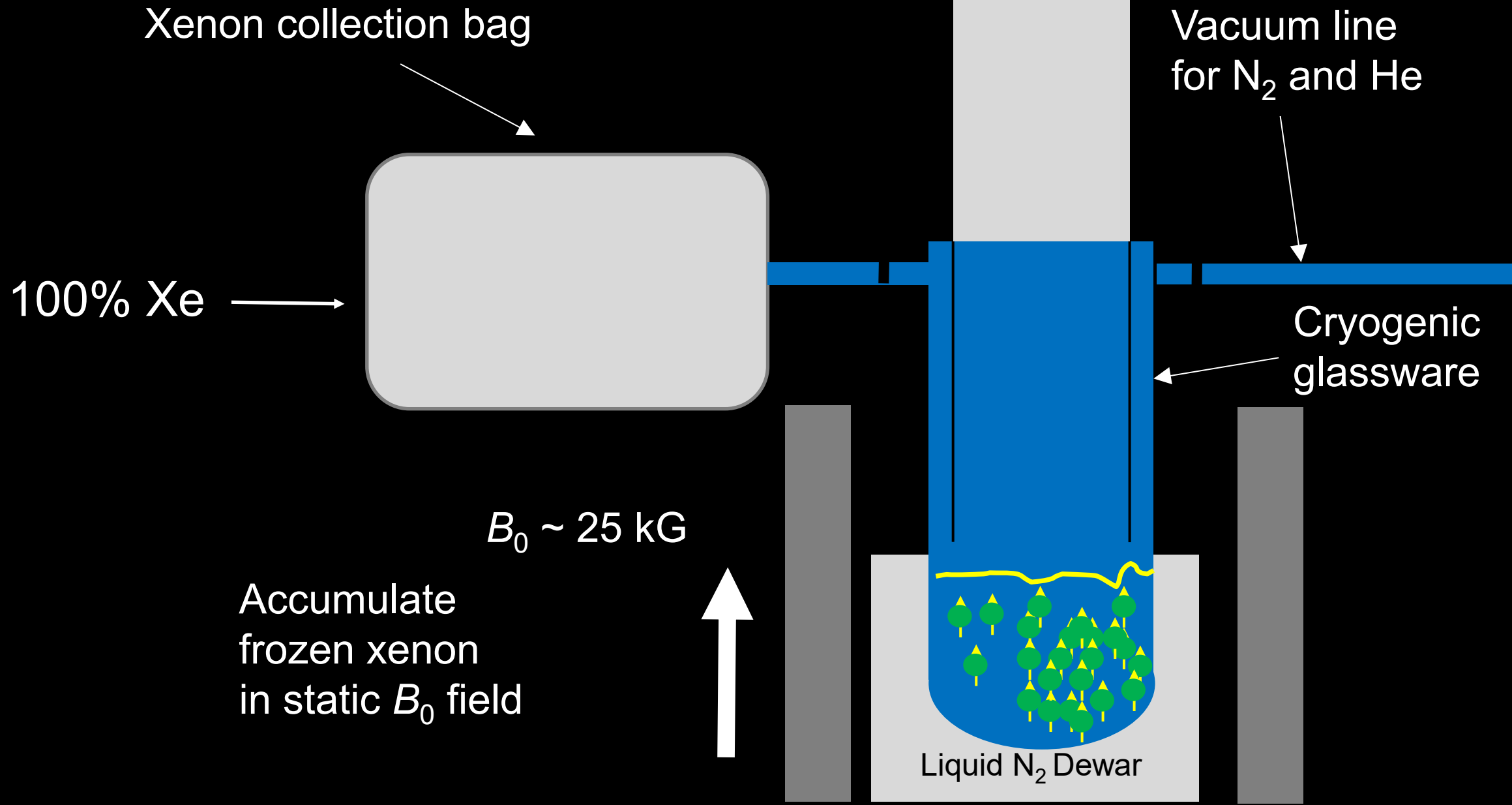
Rb vapour density curve

$T > 40^\circ\text{C}$
(313.15 K)

$$H = A\mathbf{I} \cdot \mathbf{S} + \gamma\mathbf{N} \cdot \mathbf{S} + \alpha\mathbf{K} \cdot \mathbf{S} + \dots$$

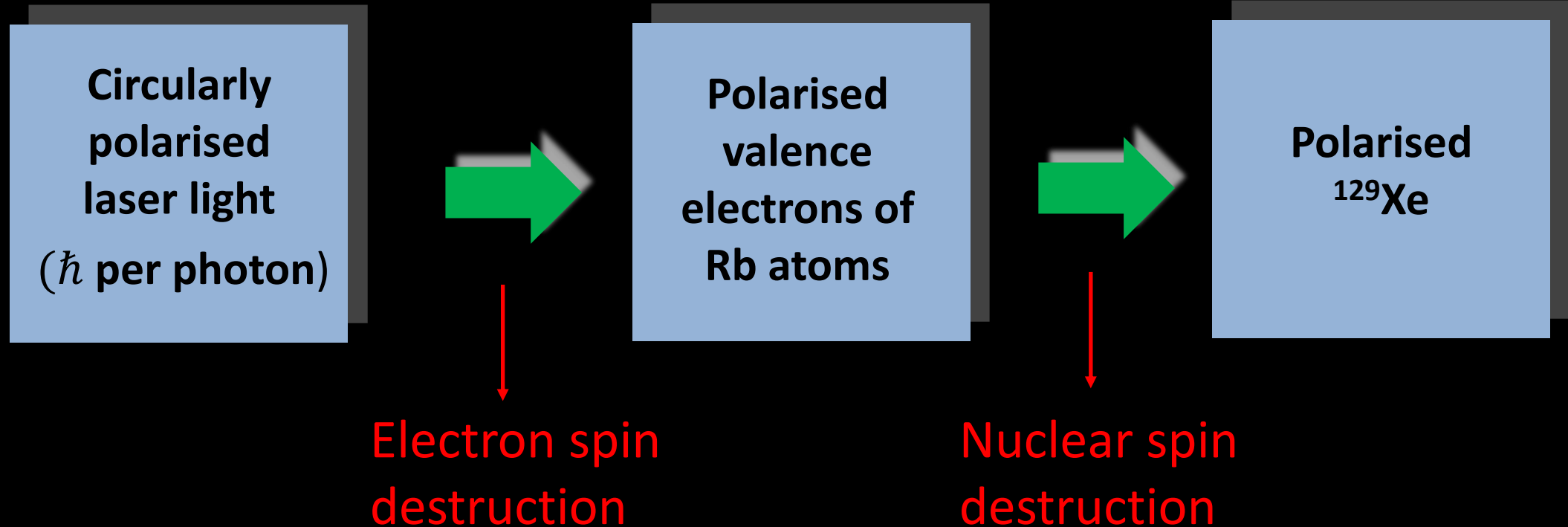
High Rb ^{129}Xe -Rb optical exchange cross section

Freeze/thaw process



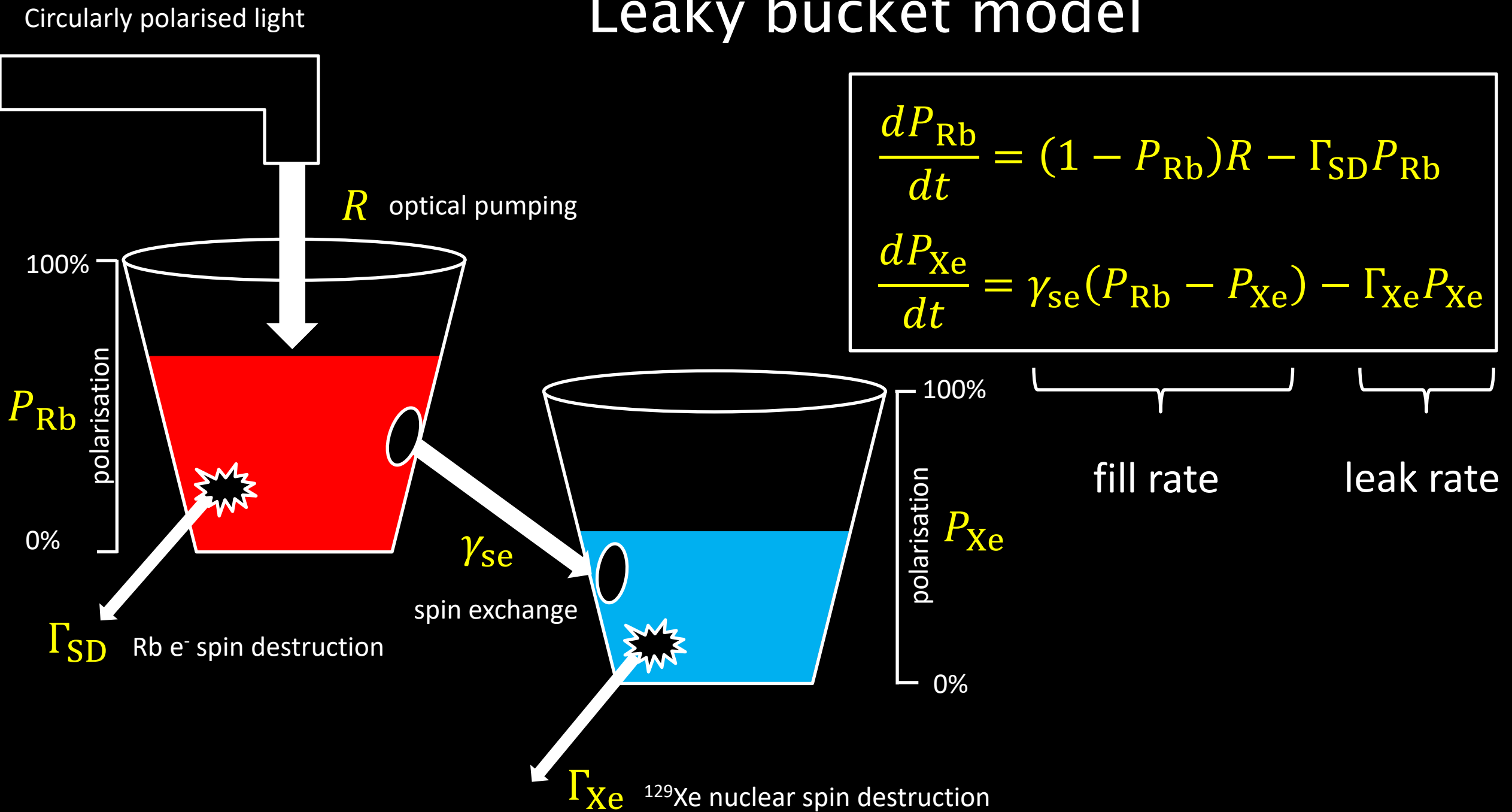
SPIN DYNAMICS OF ^{129}Xe -Rb SEOP

Angular momentum transfer in SEOP



Ideally, each laser photon flips one ^{129}Xe spin (100% efficiency).
In reality, angular momentum leaks from both Rb and Xe

Leaky bucket model



P_{Rb} and P_{Xe} time dependence

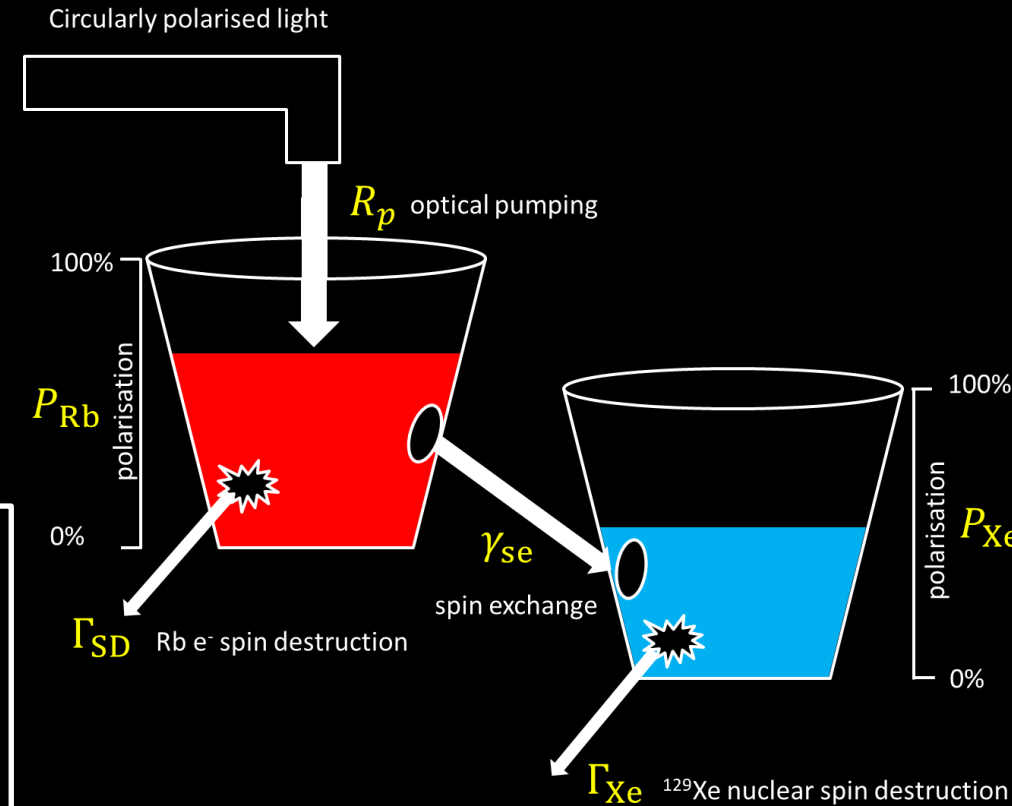
$$\frac{dP_{\text{Rb}}}{dt} = (1 - P_{\text{Rb}})R - \Gamma_{\text{SD}}P_{\text{Rb}}$$

$$\frac{dP_{\text{Xe}}}{dt} = \gamma_{\text{se}}(P_{\text{Rb}} - P_{\text{Xe}}) - \Gamma_{\text{Xe}}P_{\text{Xe}}$$

$$P_{\text{Rb}}(t) = \frac{R}{R + \Gamma_{\text{SD}}} (1 - e^{-(R + \Gamma_{\text{SD}})t})$$

$$P_{\text{Xe}}(t) = \frac{\gamma_{\text{se}}}{\gamma_{\text{se}} + \Gamma_{\text{Xe}}} P_{\text{Rb}}(t) (1 - e^{-(\gamma_{\text{se}} + \Gamma_{\text{Xe}})t})$$

Leaky bucket model



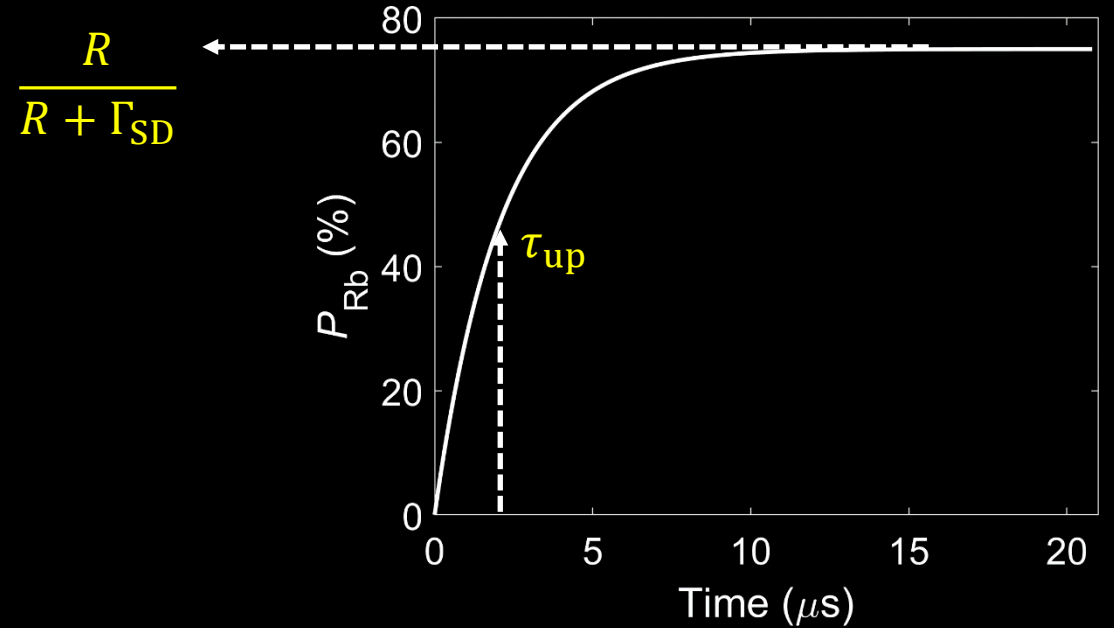
P_{Rb} and P_{Xe} steady-state and build up

Rb polarisation

$$P_{\text{Rb}}(t) = \frac{R}{R + \Gamma_{\text{SD}}} \left(1 - e^{-(R_p + \Gamma_{\text{SD}})t} \right)$$

$$\text{Steady-state: } P_{\text{Rb}} = \frac{R}{R + \Gamma_{\text{SD}}}$$

$$\text{Spin-up time: } \tau_{\text{up}} = 1/(R_p + \Gamma_{\text{SD}}) \approx \text{micro seconds}$$

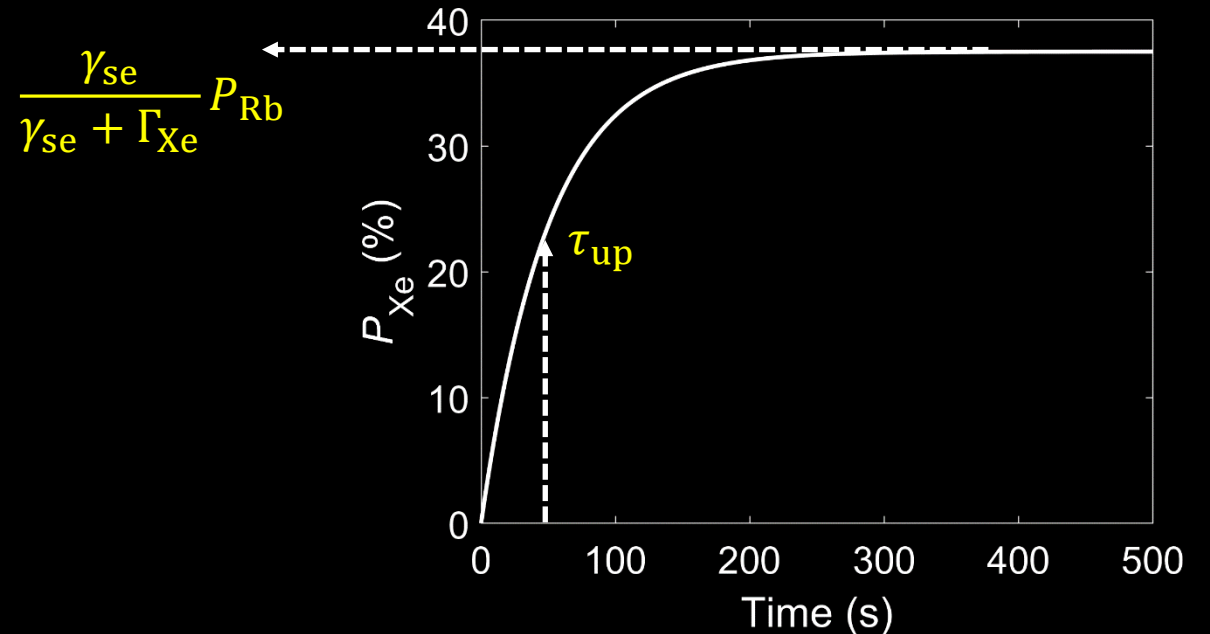


^{129}Xe polarisation

$$P_{\text{Xe}}(t) = \frac{\gamma_{\text{se}}}{\gamma_{\text{se}} + \Gamma_{\text{Xe}}} P_{\text{Rb}}(t) \left(1 - e^{-(\gamma_{\text{se}} + \Gamma_{\text{Xe}})t} \right)$$

$$\text{Steady-state: } P_{\text{Xe}} = \frac{\gamma_{\text{se}}}{\gamma_{\text{se}} + \Gamma_{\text{Xe}}} P_{\text{Rb}}$$

$$\text{Spin-up time: } \tau_{\text{up}} = 1/(\gamma_{\text{se}} + \Gamma_{\text{Xe}}) \approx 10\text{s of seconds}$$

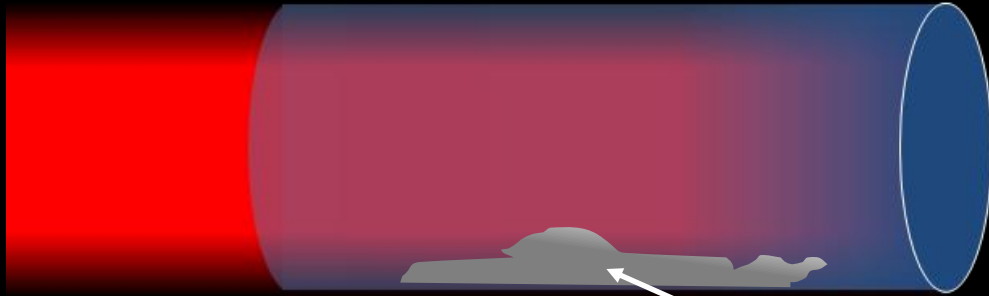


OPTIMISING LIGHT PROPAGATION

Light propagation

Photon flux Φ

→ z



Rb pool

$$\frac{\partial \Phi(\nu, z)}{\partial z} = - \underbrace{\lambda^{-1}(\nu, z)}_{\text{absorption length per photon}} \Phi(\nu, z)$$

λ = absorption length
per photon

$$\lambda^{-1}(\nu, z) = [\text{Rb}] \sigma(\nu) [1 - P_{\text{Rb}}(z)]$$

↑
Rb vapour density

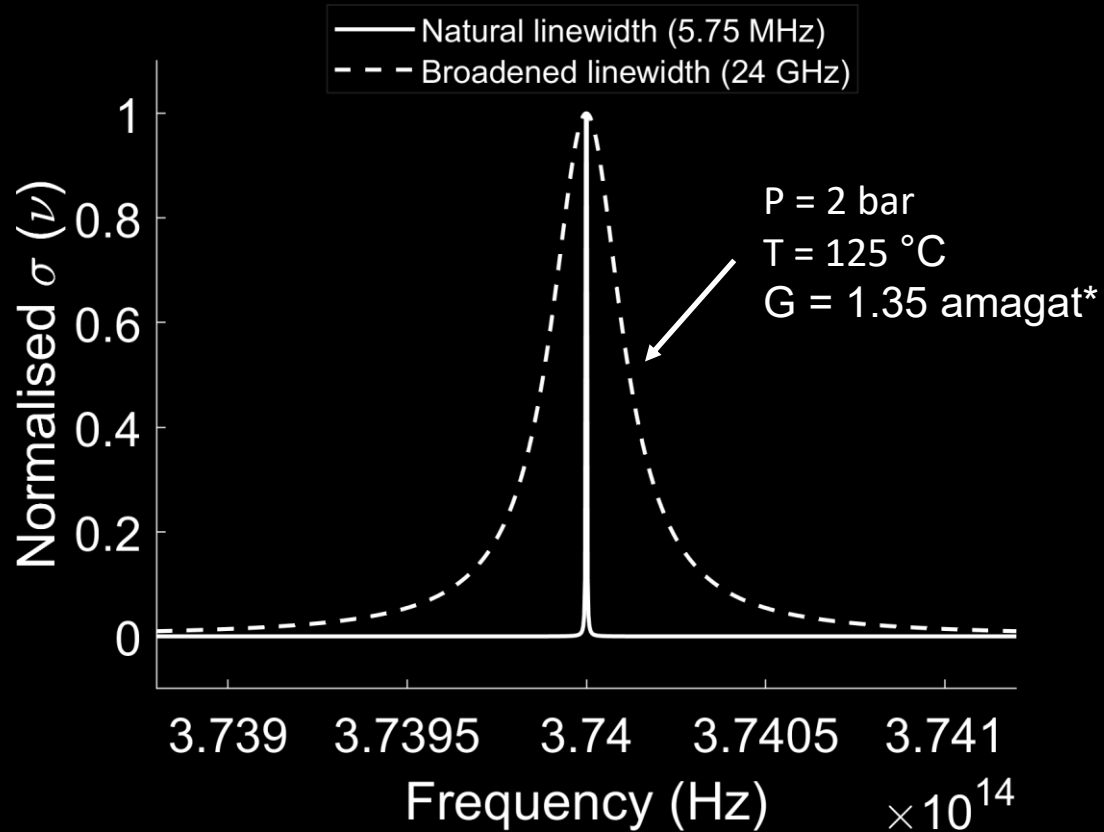
← Rb polarisation

← Rb D1 line absorption profile

$$\frac{\partial \Phi(\nu, z)}{\partial z} = - [\text{Rb}] \sigma(\nu) [1 - P_{\text{Rb}}(z)] \Phi(\nu, z)$$

Role of buffer gases N₂ and He

Pressure broadening of D₁ line

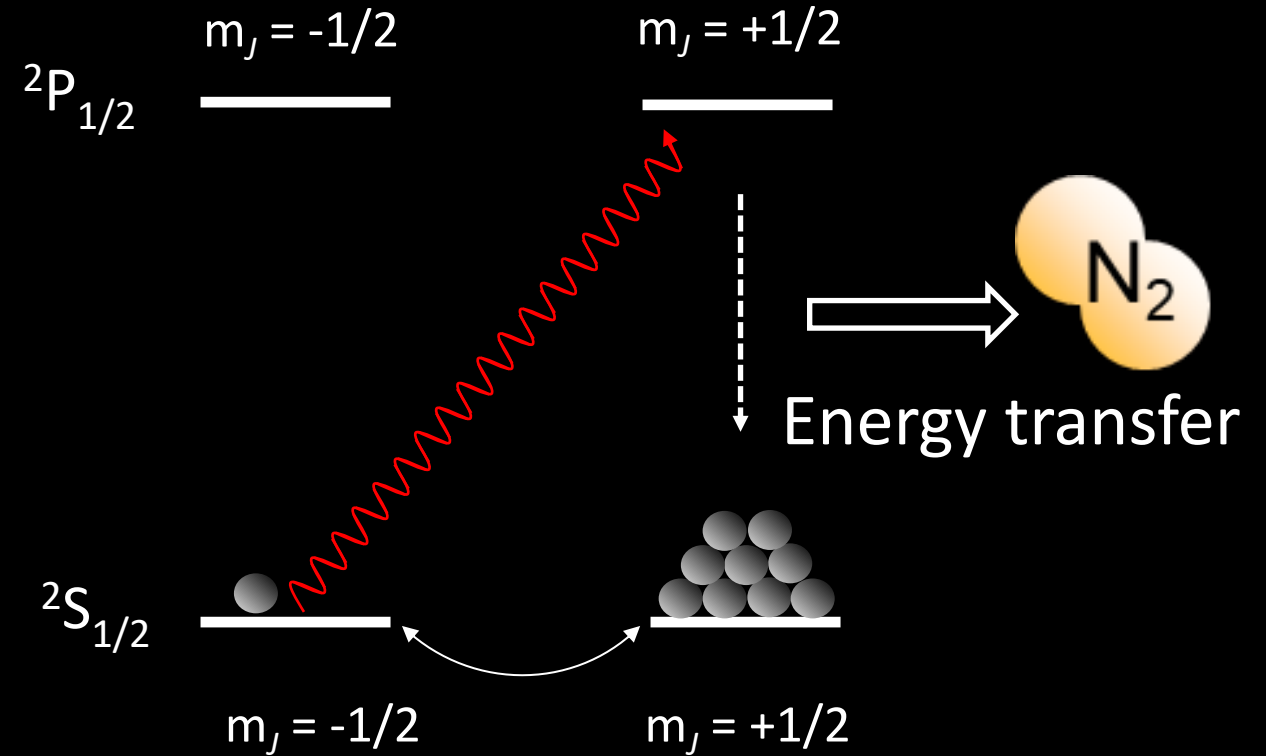


He/N₂ : $\Delta\nu_a \sim 18 \text{ GHz/amagat}$

Romalis, PRA(56), 1997

*1 amagat = gas number density at STP ($T = 0^\circ\text{C}$ and $P = 1 \text{ atm}$)

Non-radiative decay (quenching)

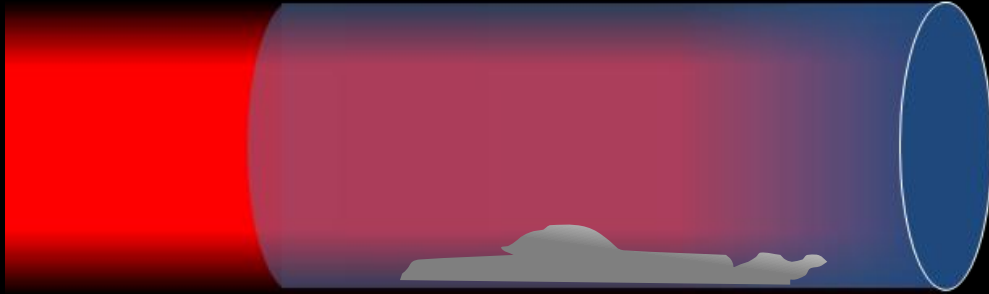


Wagshul and Chupp, PRA(40), 1989

Absorption profile over cell length

Photon flux Φ

→ z

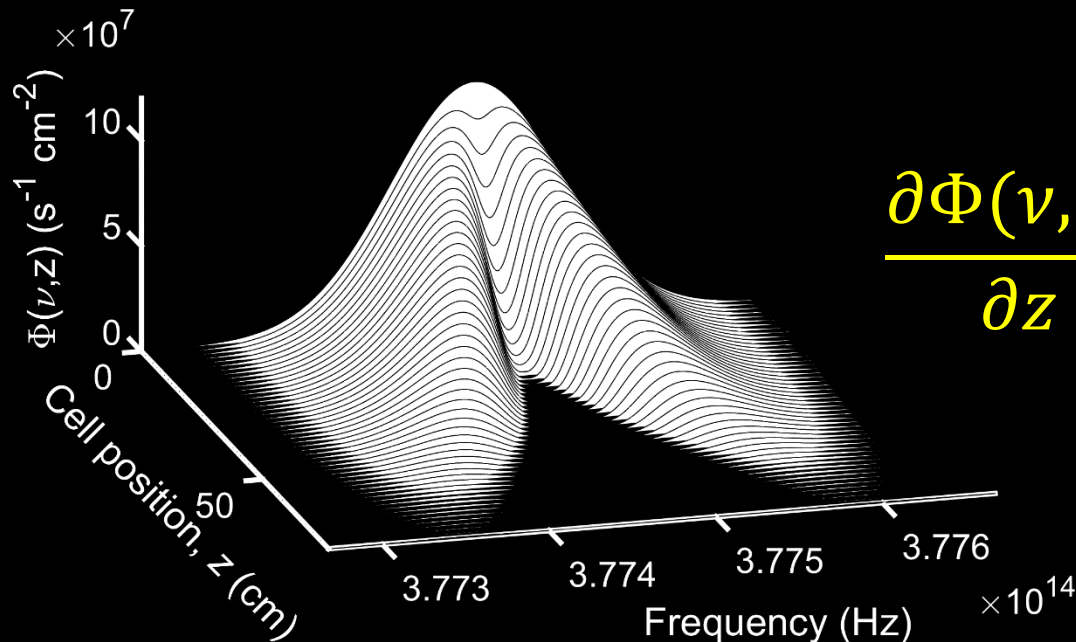


Incident flux

$$\Phi(\nu, 0) = \Phi_0 \exp \left[-4 \ln 2 \frac{(\nu - \nu_l)^2}{\Delta \nu_l^2} \right] \quad \text{Gaussian}$$

Absorption

$$\sigma(\nu) = \sigma_0 \frac{\Delta \nu_a / 2\pi}{(\nu - \nu_a)^2 + \left(\frac{\Delta \nu_a}{2} \right)^2} \quad \text{Lorentzian}$$



$$\frac{\partial \Phi(\nu, z)}{\partial z} = -[\text{Rb}] \sigma(\nu) [1 - P_{\text{Rb}}(z)] \Phi(\nu, z)$$

$$\Delta \nu_l = 142 \text{ GHz (0.30 nm)}$$

$$\Delta \nu_a = 24 \text{ GHz (0.05 nm)}$$

Light propagation link to optical pumping

Photon flux Φ



$$R(z) = \int \Phi(\nu, z) \sigma(\nu) d\nu$$

Optical pumping rate

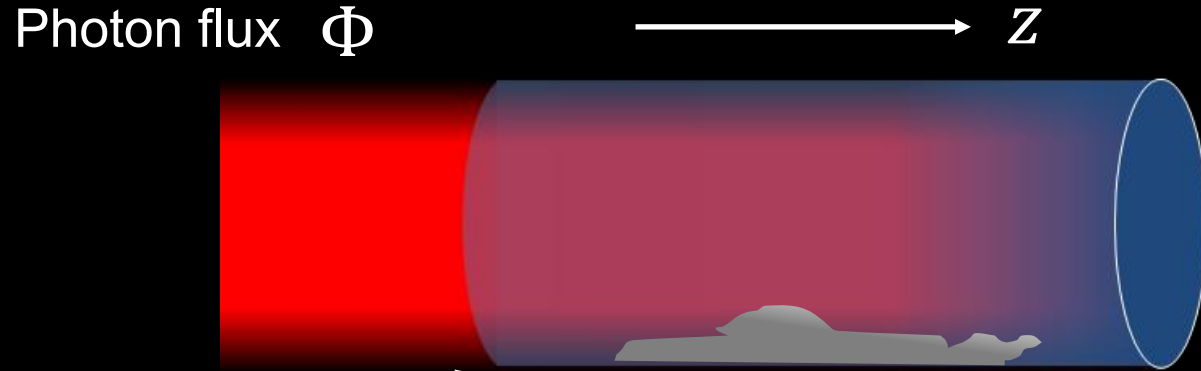
$$\frac{\partial \Phi(\nu, z)}{\partial z} = -[R_b] \sigma(\nu) [1 - P_{R_b}(z)] \Phi(\nu, z)$$

$$\frac{d\Phi(z)}{dz} = \int \frac{\partial \Phi(\nu, z)}{\partial z} d\nu = -[R_b] [1 - P_{R_b}(z)] \int \Phi(\nu, z) \sigma(\nu) d\nu$$

$$\frac{d\Phi(z)}{dz} = -[R_b] [1 - P_{R_b}(z)] R(z)$$

Relates photon attenuation
with pumping rate

Optical pumping rate vs. cell length



$$\frac{d\Phi(z)}{dz} = -[\text{Rb}][1 - P_{\text{Rb}}(z)]R(z)$$

$$R_0(\nu, 0) = \int_{-\infty}^{\infty} \sigma(\nu)\Phi(\nu) = \alpha\Phi$$

$$\alpha = \frac{2\sqrt{\pi \ln 2} r_e f \lambda_l^3 w'(r, s)}{hc\Delta\lambda n_p}$$

Appelt, PRA(52), 1998

$$\frac{dR(z)}{dz} = -[\text{Rb}]\alpha[1 - P_{\text{Rb}}(z)]R(z)$$

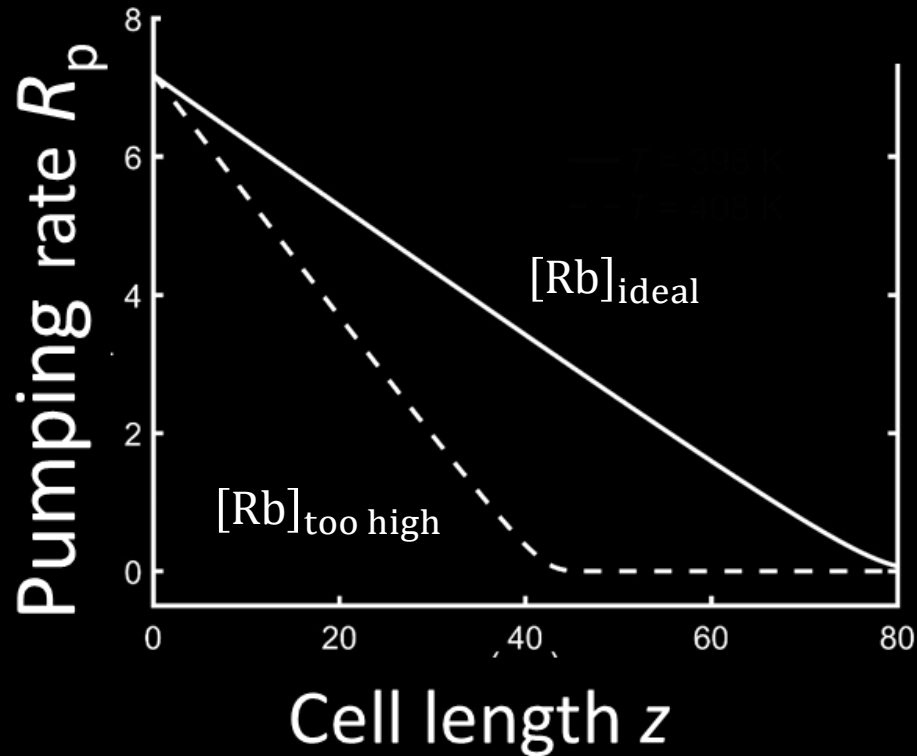
$$W(f(x)) = x, \text{ for } f(x) = xe^x$$

$$R(z) = \Gamma_{SD} W \left(\frac{R_0}{\Gamma_{SD}} \exp \left(\frac{R_0}{\Gamma_{SD}} - \alpha[\text{Rb}]z \right) \right)$$

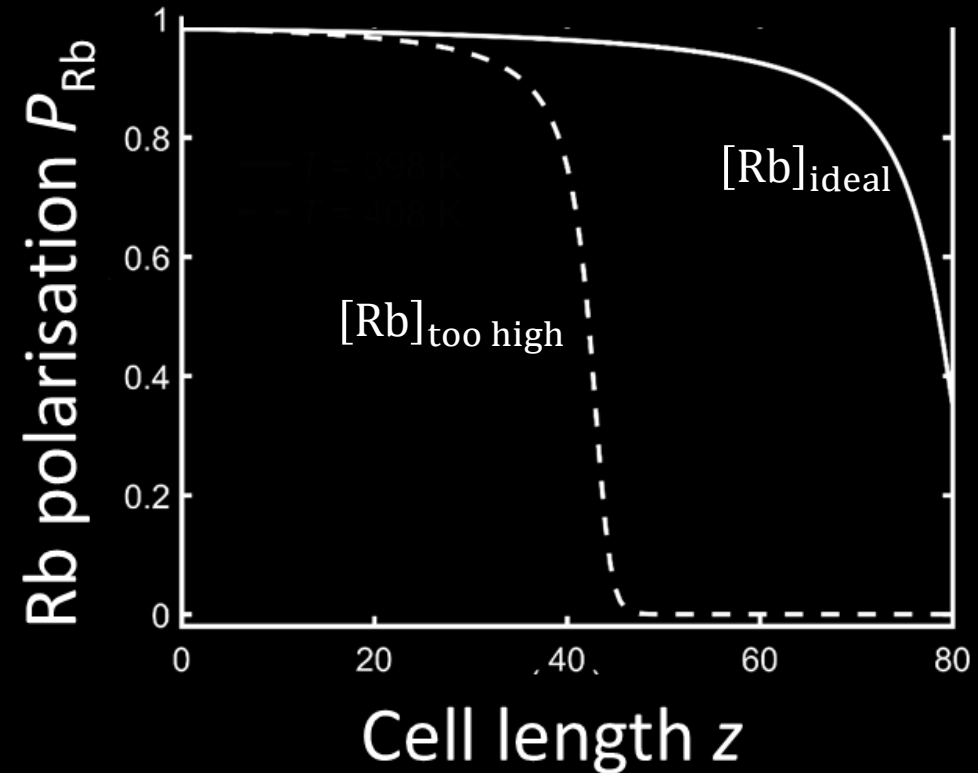
Product log
function

Optimisation tools: Light propagation, R_p and P_{Rb}

$$R(z) = \Gamma_{SD} W \left(\frac{R_0}{\Gamma_{SD}} \exp \left(\frac{R_0}{\Gamma_{SD}} - \alpha[Rb]z \right) \right)$$



$$P_{Rb}(z) = \frac{R(z)}{R(z) + \Gamma_{SD}}$$

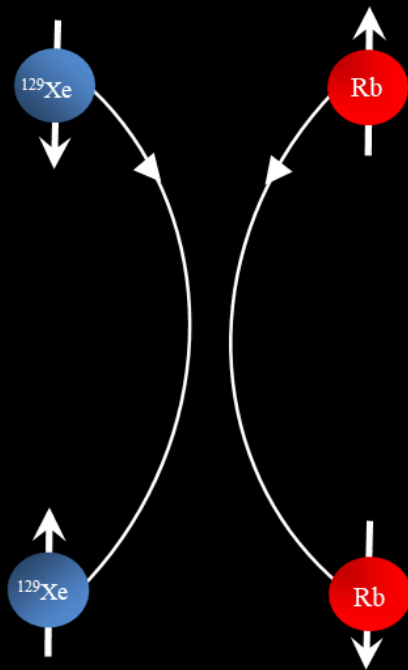


Solid white line necessary for high average P_{Rb} over the cell volume

^{129}Xe POLARISATION OPTIMISATION TOOLS

^{129}Xe -Rb spin exchange

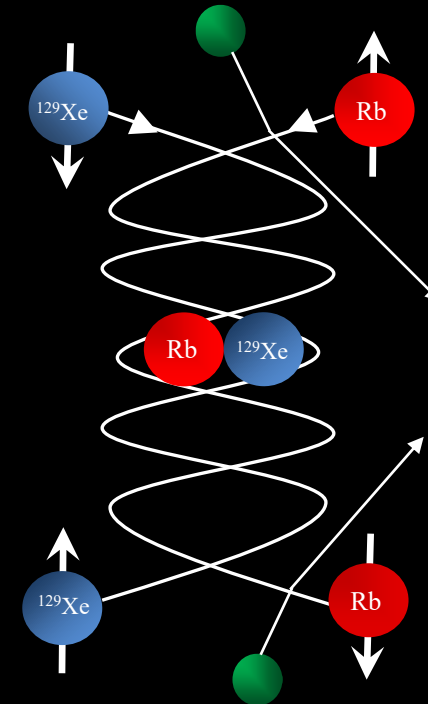
Two-body collisional exchange



- Simple two-body cross section
- Independent of P_{Rb} and gas composition

Three-body vdW molecular exchange

3rd body {N₂, He, Xe}



- Complicated cross section
- Depends on P_{Rb} and gas composition

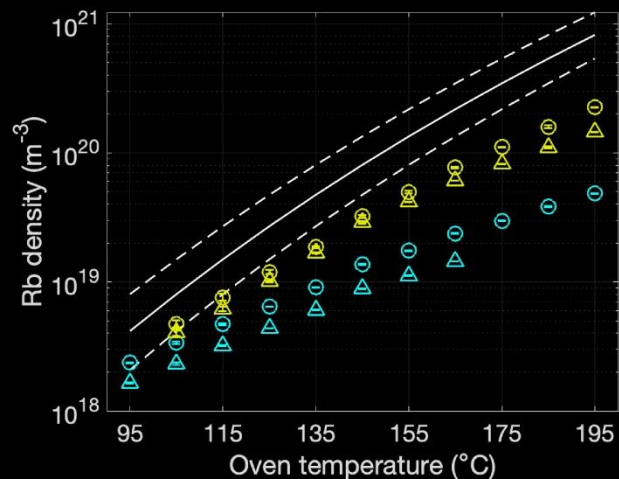
^{129}Xe -Rb spin exchange

Two-body collisional exchange

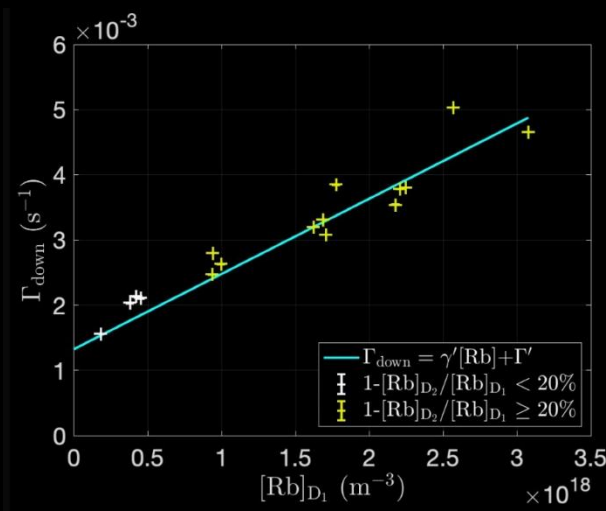
$$\gamma_{se}^{bc} = \langle \sigma v \rangle [\text{Rb}]$$

Binary spin-exchange cross section

Ball et al, Molecules(8), 2023



Factor-2 lower [Rb] than standard saturation curves



$$\gamma' = \langle \sigma v \rangle + \gamma'_{vdW} = 1.2 \times 10^{-21} \text{ cm}^3 \text{ s}^{-1}$$

Literature: $\langle \sigma v \rangle = 0.1 \times 10^{-21}$ to $1 \times 10^{-21} \text{ cm}^3 \text{ s}^{-1}$

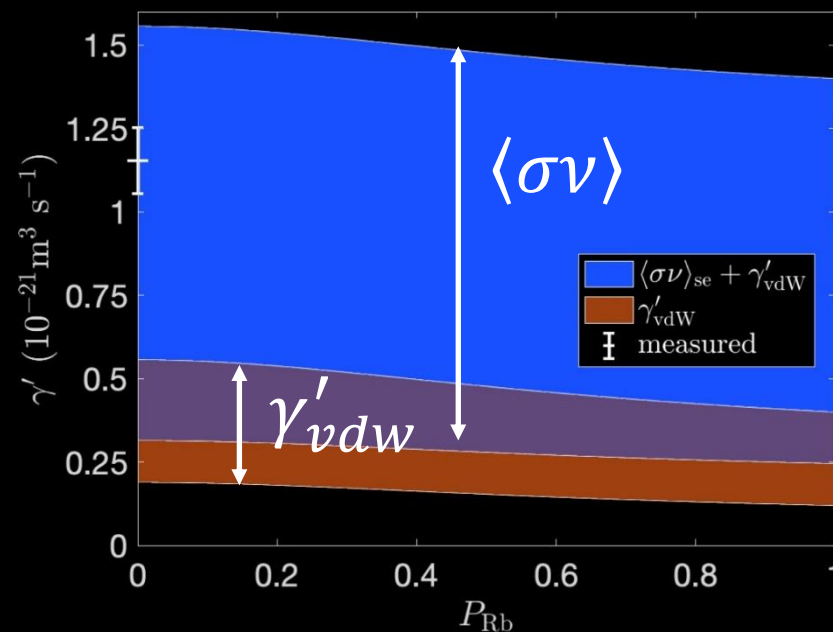
Factor-10 range in values...

Three-body vdW molecular exchange

$$\gamma_{se}^{vdw} = \frac{1}{2T_K} \left(\frac{\omega_{sr} \tau}{x} \right)^2 \sum_i \eta_i \left(\frac{1 + q_i (\omega_{h,i} \tau)^2 / [I_i]^2}{1 + (\omega_{h,i} \tau)^2} \right) = \gamma'_{vdW} [\text{Rb}]$$

τ = molecular lifetime ← Gas composition dependent

$q_i = 1 + \epsilon(I, P_{\text{Rb}})$ ← Nuclear slowing down factor – depends on P_{Rb}

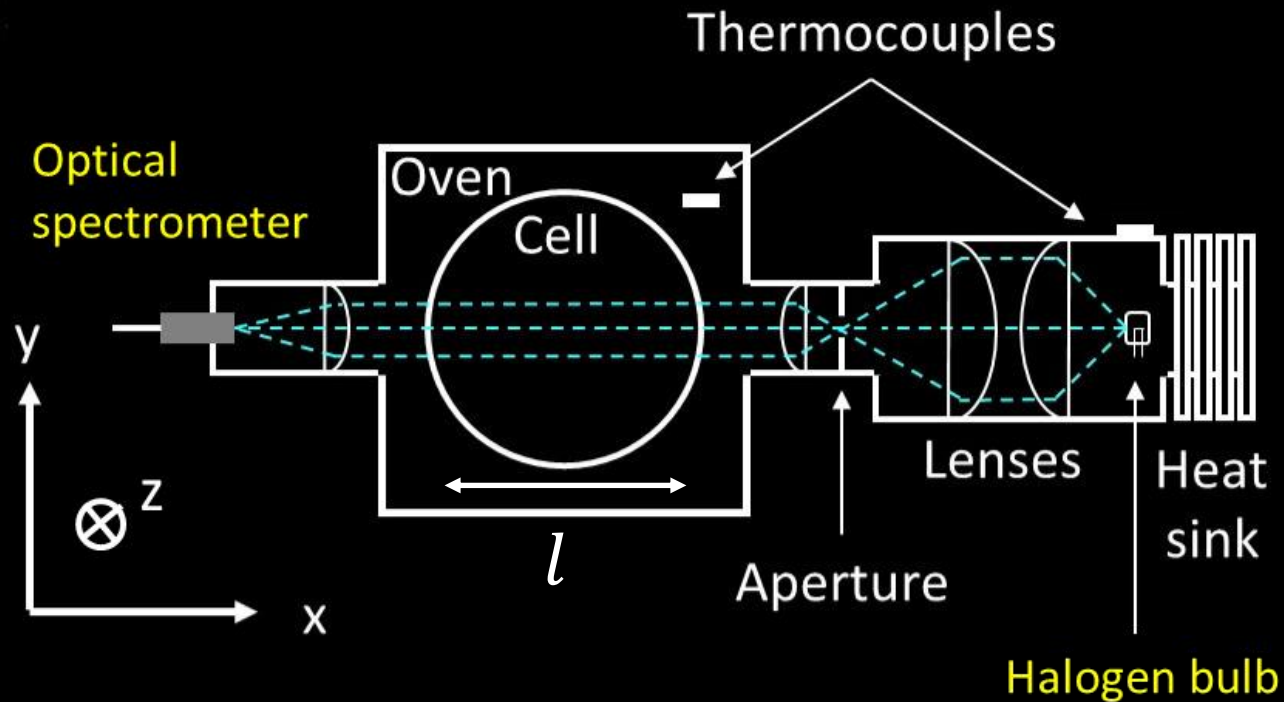


Ball et al, Molecules(8), 2023

Measuring Rb vapour density

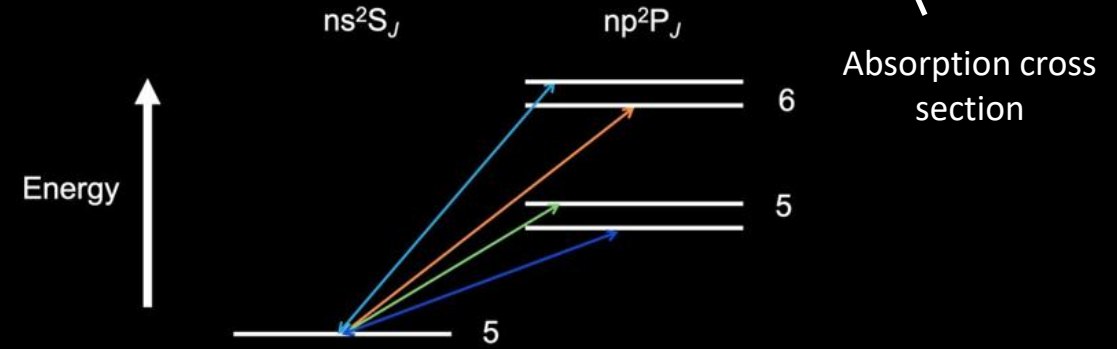
Atomic Absorption spectroscopy

Experimental setup



Beer-Lambert law

$$I(\nu) = I_0 e^{-[\text{Rb}] \sigma(\nu) l}$$



Transition	Wavelength (nm)	Oscillator strength, f
$5^2S_{1/2} \rightarrow 6^2P_{1/2}$	422	3.87×10^{-3}
$5^2S_{1/2} \rightarrow 6^2P_{3/2}$	420	9.46×10^{-3}
$5^2S_{1/2} \rightarrow 5^2P_{1/2} (D_1)$	795	3.422×10^{-1}
$5^2S_{1/2} \rightarrow 5^2P_{3/2} (D_2)$	780	6.957×10^{-1}

Measuring Rb vapour density

Atomic Absorption spectroscopy

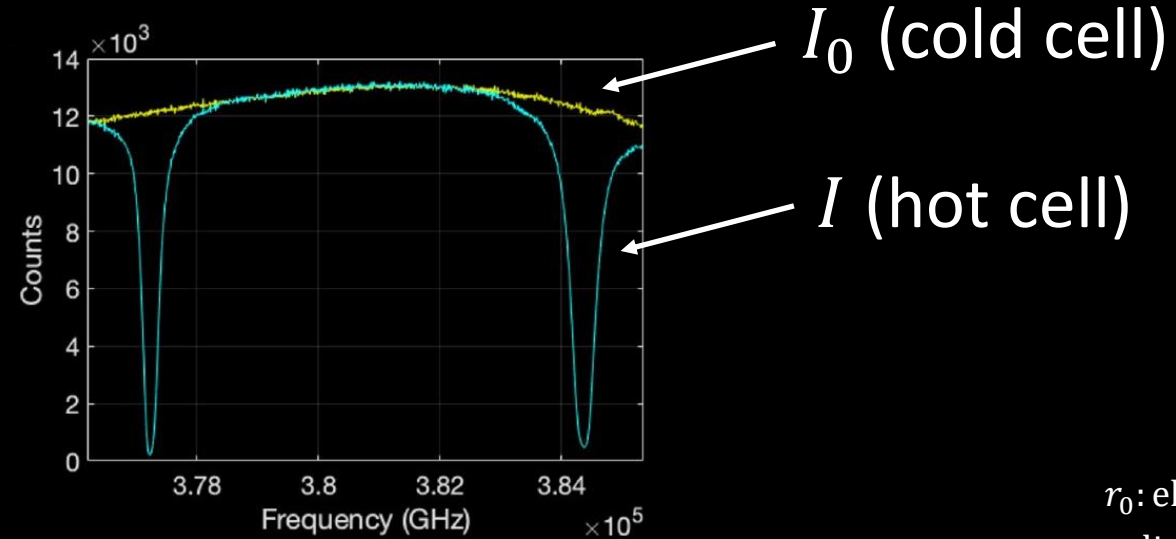
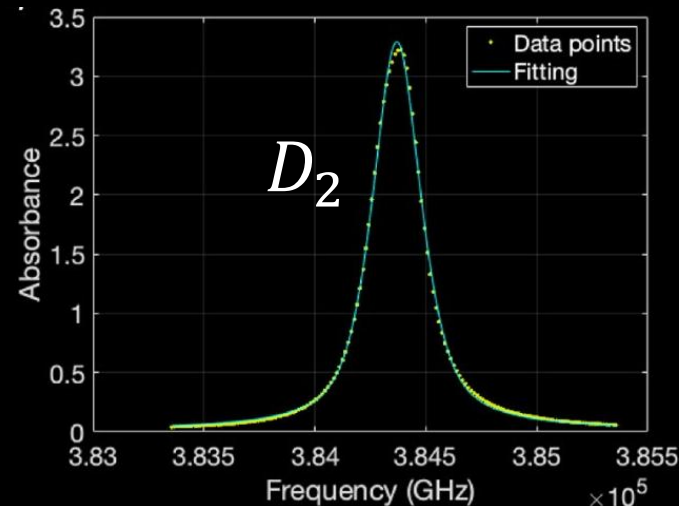
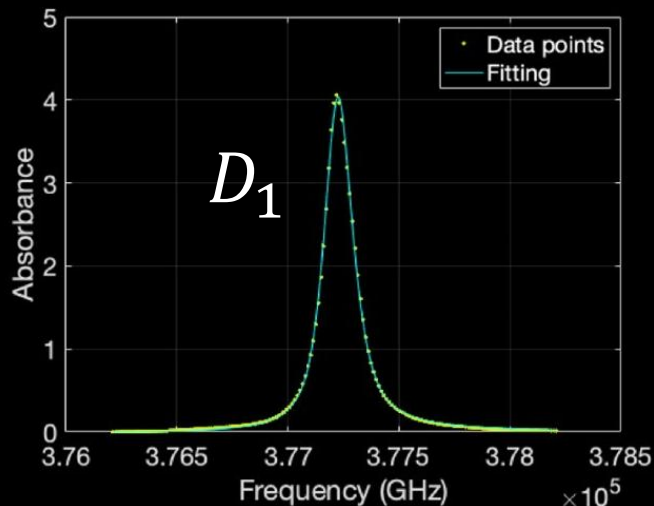
$$I = I_0 e^{-[\text{Rb}]\sigma(\nu)l}$$

Absorbance

Amplitude

$$S(\nu) = \ln\left(\frac{I_0}{I}\right) = AL(\nu)$$

Normalised Lorentzian



Transition oscillator strength

r_0 : electron radius
 c : light speed

$$[\text{Rb}] = \frac{1}{\sigma_0 l} \int S(\nu) d\nu$$

$$\sigma_0 = \int \sigma(\nu) d\nu = \pi r_0 c f$$

$$[\text{Rb}] = \frac{A}{\pi r_0 c f l}$$

Optimisation tools: ^{129}Xe polarisation

$$P_{\text{Xe}}(t_{\text{res}}) = \frac{\gamma_{\text{se}}}{\gamma_{\text{se}} + \Gamma_{\text{Xe}}} \langle P_{\text{Rb}} \rangle [1 - e^{-t_{\text{res}}/\tau_{\text{up}}}]$$

Diagram illustrating the equation for ^{129}Xe polarisation, with arrows indicating the physical parameters and their relationships:

- $\langle P_{\text{Rb}} \rangle$: mean Rb polarisation over cell volume
- t_{res} : Xe cell residency time
- τ_{up} : ^{129}Xe spin-up time
- Γ_{Xe} : ^{129}Xe spin-destruction rate
- γ_{se} : ^{129}Xe spin-exchange rate

Relationships and definitions:

- $\gamma_{\text{se}} = \gamma_{\text{se}}^{bc} + \gamma_{\text{se}}^{vdW}$
- $\gamma_{\text{se}} \propto [\text{Rb}]$
- $\Gamma_{\text{Xe}} = 1/T_1$
- $\tau_{\text{up}} = 1/(\gamma_{\text{se}} + \Gamma_{\text{Xe}})$

For high P_{Xe} :

$$\gamma_{\text{se}} > 1/T_1 \quad \text{High } \langle P_{\text{Rb}} \rangle \quad t_{\text{res}} > \tau_{\text{up}}$$

Optimisation tools: Xe volume production Q_{Xe}

$$\gamma_{\text{se}} > 1/T_1 \quad \text{High } \langle P_{\text{Rb}} \rangle \quad t_{\text{res}} > \tau_{\text{up}}$$

$$P_{\text{Xe}}(t_{\text{res}}) = \frac{\gamma_{\text{se}}}{\gamma_{\text{se}} + \Gamma_{\text{Xe}}} \langle P_{\text{Rb}} \rangle [1 - e^{-t_{\text{res}}/\tau_{\text{up}}}]$$

$$Q_{\text{Xe}} = [\text{Xe}]V_{\text{cell}}/t_{\text{res}} \quad \text{Xe volume production rate}$$

Stopped-flow: Colder cell increase T_1 , giving higher P_{Xe} ; Colder cell, longer τ_{up} : need longer t_{res} to maintain P_{Xe} which means lower production rates Q_{Xe}

Continuous-flow: High production rate Q_{Xe} due to gas flow means shorter t_{res} . Need hotter cell to reduce τ_{up} and maintain P_{Xe} . Hotter cell decreases T_1 , giving lower P_{Xe} .

Continuous-flow polariser optimisation

Community has moved towards large cells

- Long cell maximises absorption of incident photons at lower [Rb]
- Laser heating/Rb runaway less likely
- At high gas flow rate Q and lower [Rb]
 $t_{\text{res}} > \tau_{\text{up}}$ for large volume cell



$$t_{\text{res}} = \frac{[G]V_{\text{cell}}}{Q} \quad \tau_{\text{up}} \propto 1/[\text{Rb}]$$

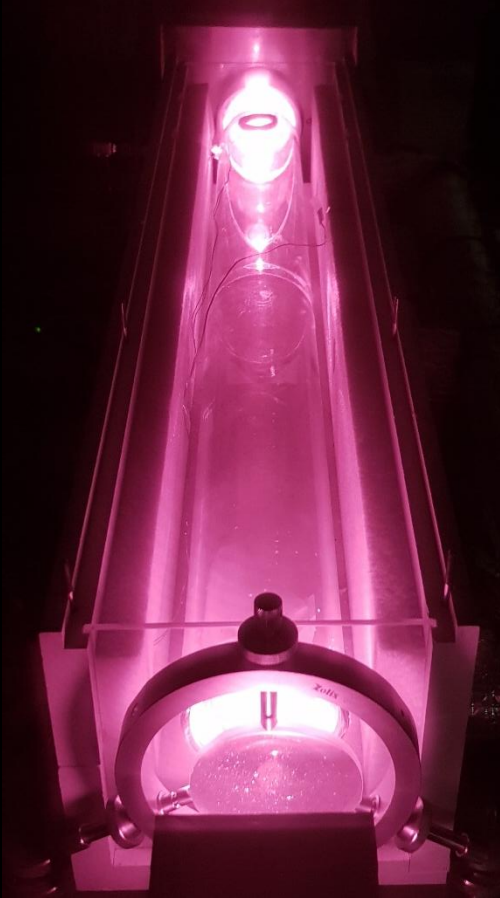
High P_{Xe} at rapid Xe production rates

Cell volume P_{Xe} simulations

$$P_{Xe}(t_{res}) = P_0(1 - e^{-t_{res}/\tau_{up}})$$

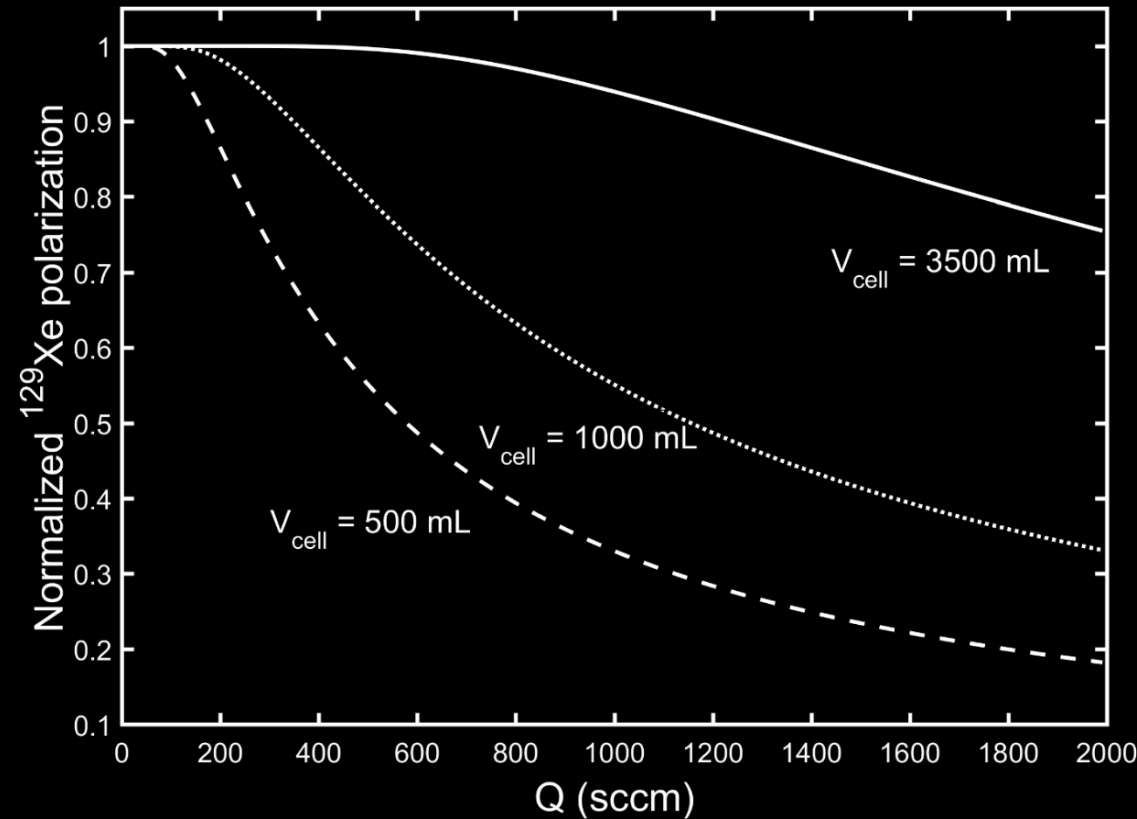
$$P_{Xe}(Q) = P_0(1 - e^{-[G]V_{cell}/Q\tau_{up}})$$

$$t_{res} = \frac{[G]V_{cell}}{Q}$$



Cell dimensions:

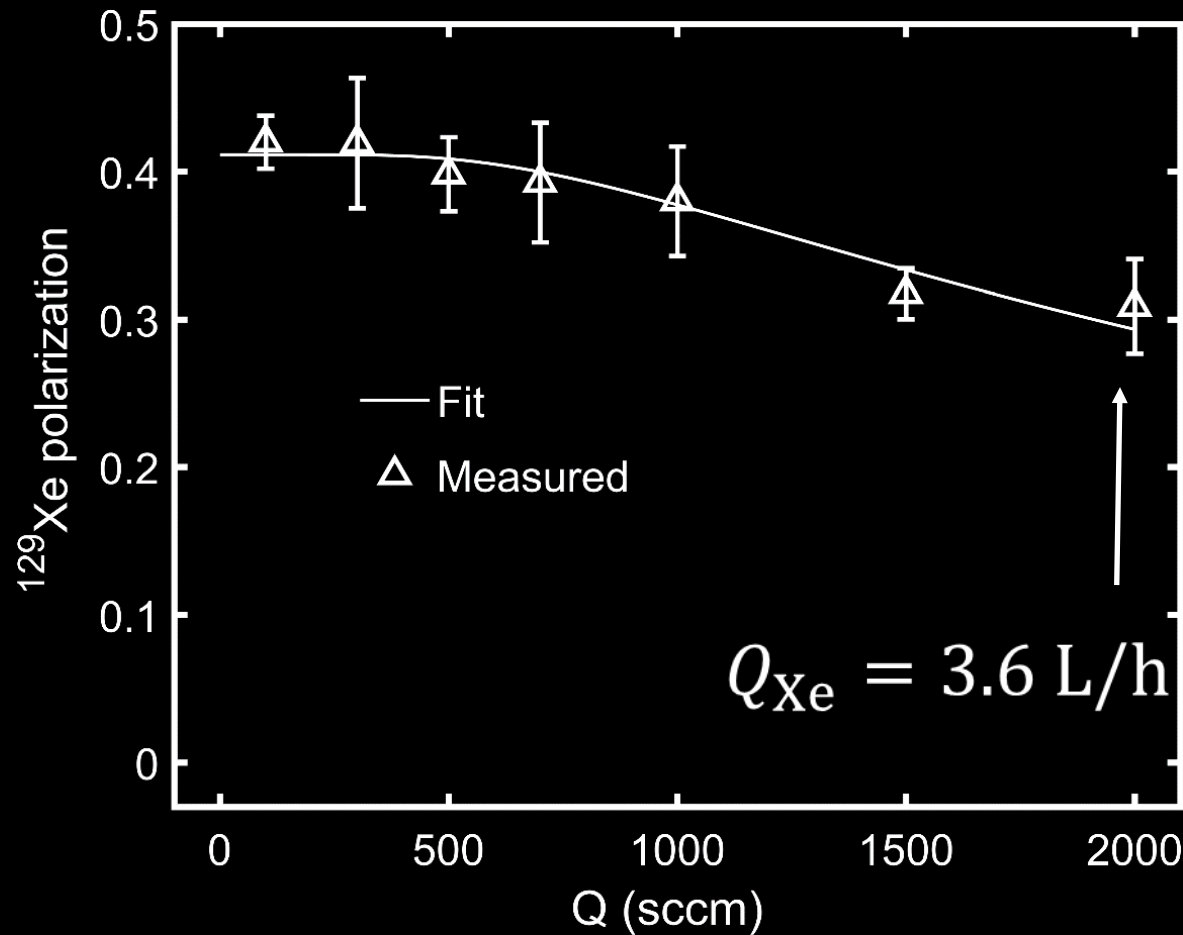
- Length = 80cm
- Diameter = 7.5 cm
- Volume = 3530 mL



Simulated:

- $T_{\text{cell}} = 398 \text{ K}$
- $P_{\text{cell}} = 1.25 \text{ bar}$
- $[G] = 0.85 \text{ amg}$

^{129}Xe polariser optimisation



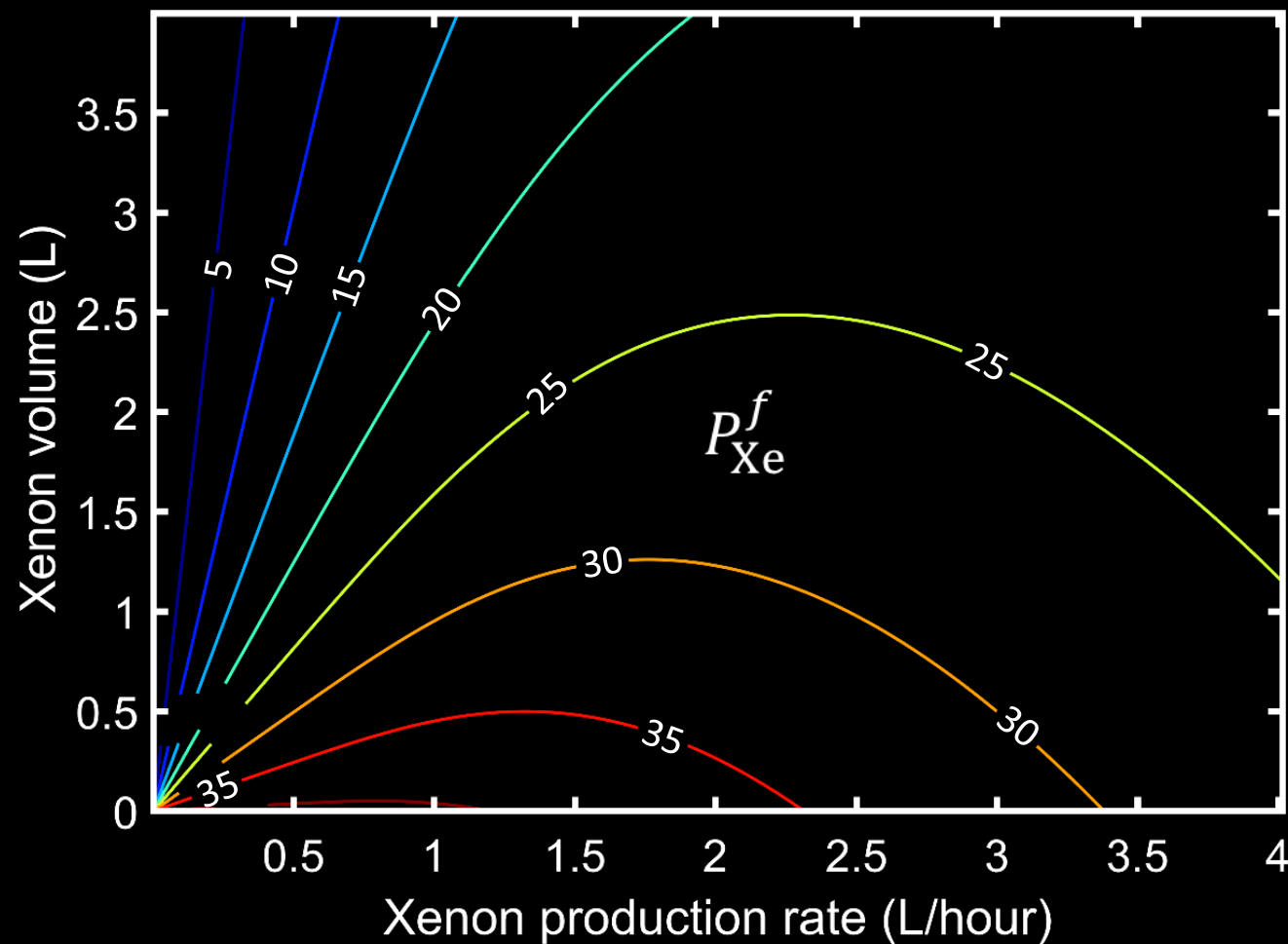
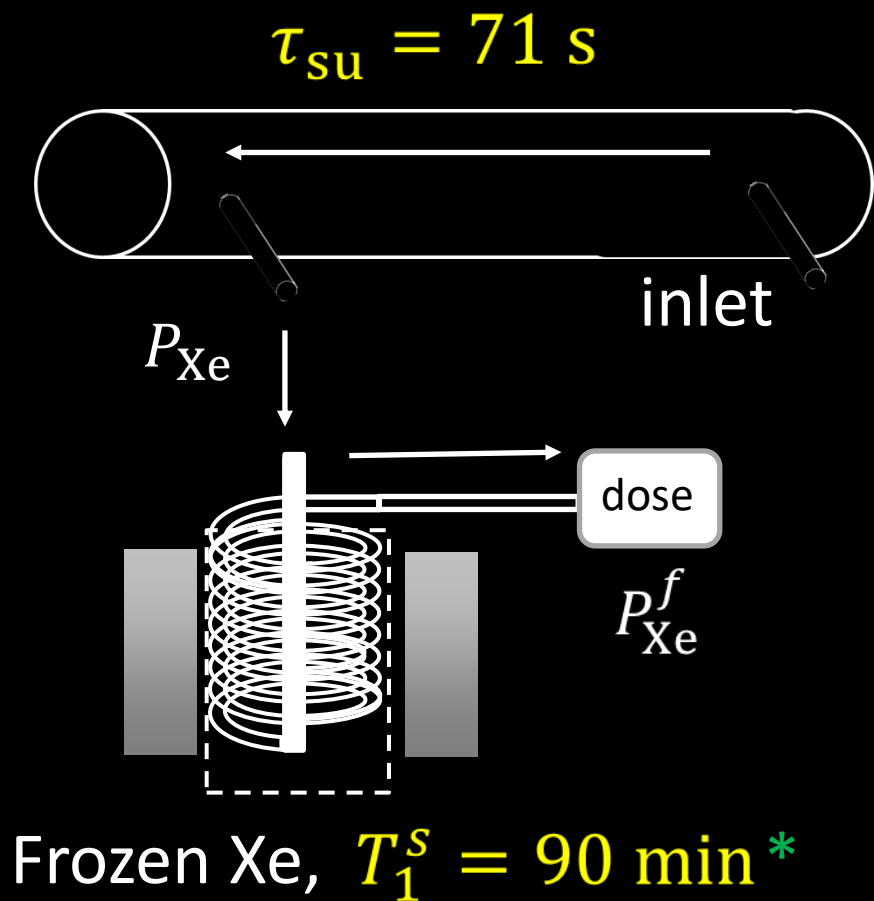
Optimised parameters:

- $T_{\text{cell}} = 398 \text{ K}$
- $P_{\text{cell}} = 1.25 \text{ bar}$
- 3% Xe gas mix
- $[G] = 0.85 \text{ amg}$
- $V_{\text{cell}} = 3530 \text{ mL}$

$$Q = 2000 \text{ sccm} \Rightarrow t_{\text{res}} = 90 \text{ s}$$

$$P_{\text{Xe}}(Q) = P_0(1 - e^{[G]V_{\text{cell}}/Q\tau_{\text{up}}}) \Rightarrow \tau_{\text{up}} = 71 \text{ s} \Rightarrow P(Q_{\text{Xe}} = 3.6 \text{ L/h}) \approx 0.75P_0$$

^{129}Xe production map



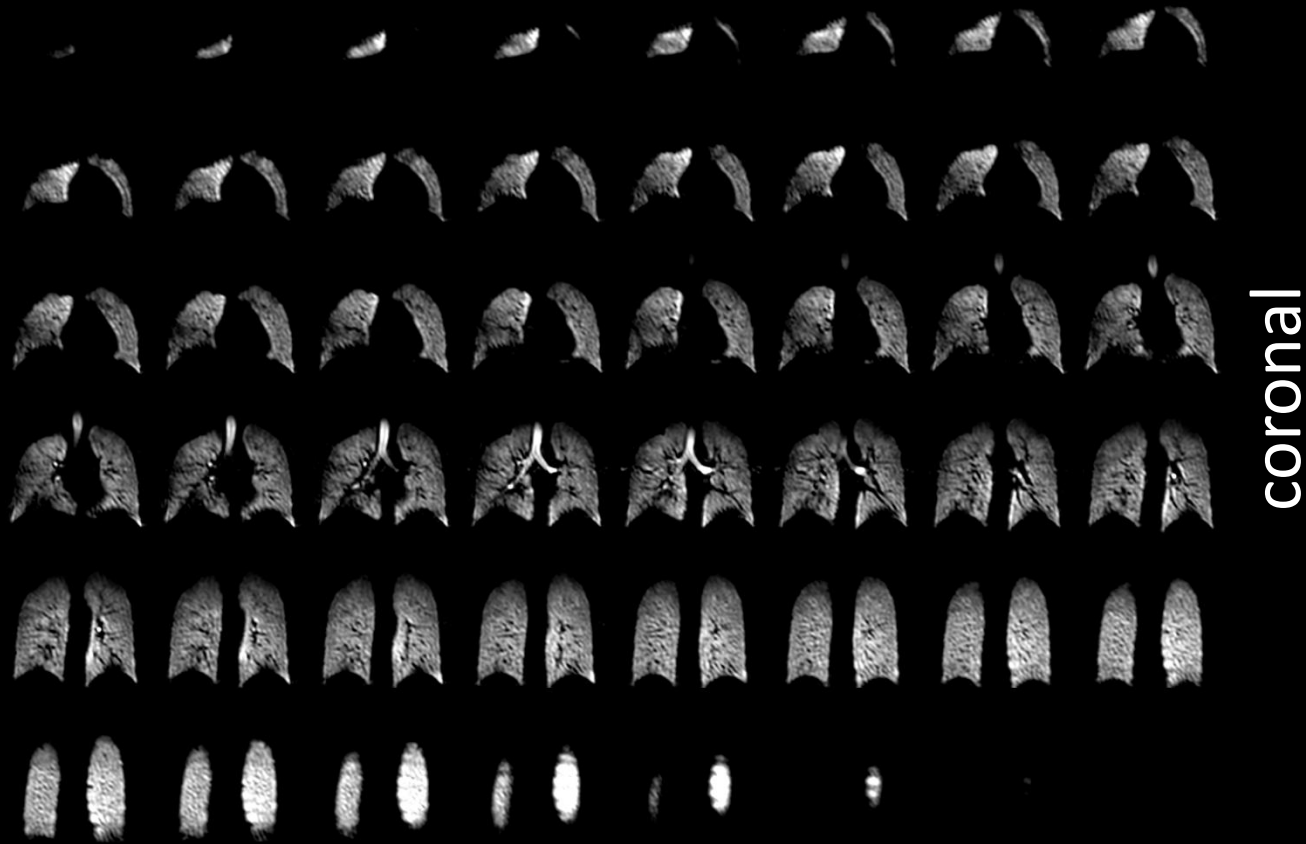
$$P_{\text{Xe}}^f(Q, t_a) = P_{\text{Xe}}(Q) \left[1 - e^{-t_a/T_1^s} \right] T_1^s / t_a$$

300 mL, P_{Xe} 30% in ~ 5 min

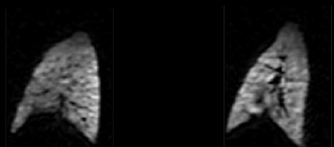
*Norquay et al., JAppl Phys(13), 2013

Norquay et al., Phys Rev Lett(121), 2018

3D ^{129}Xe human lung imaging with enriched Xe

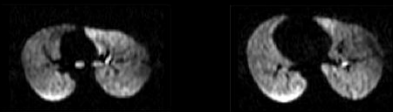


ENXe 1L dose
generated ~20 min



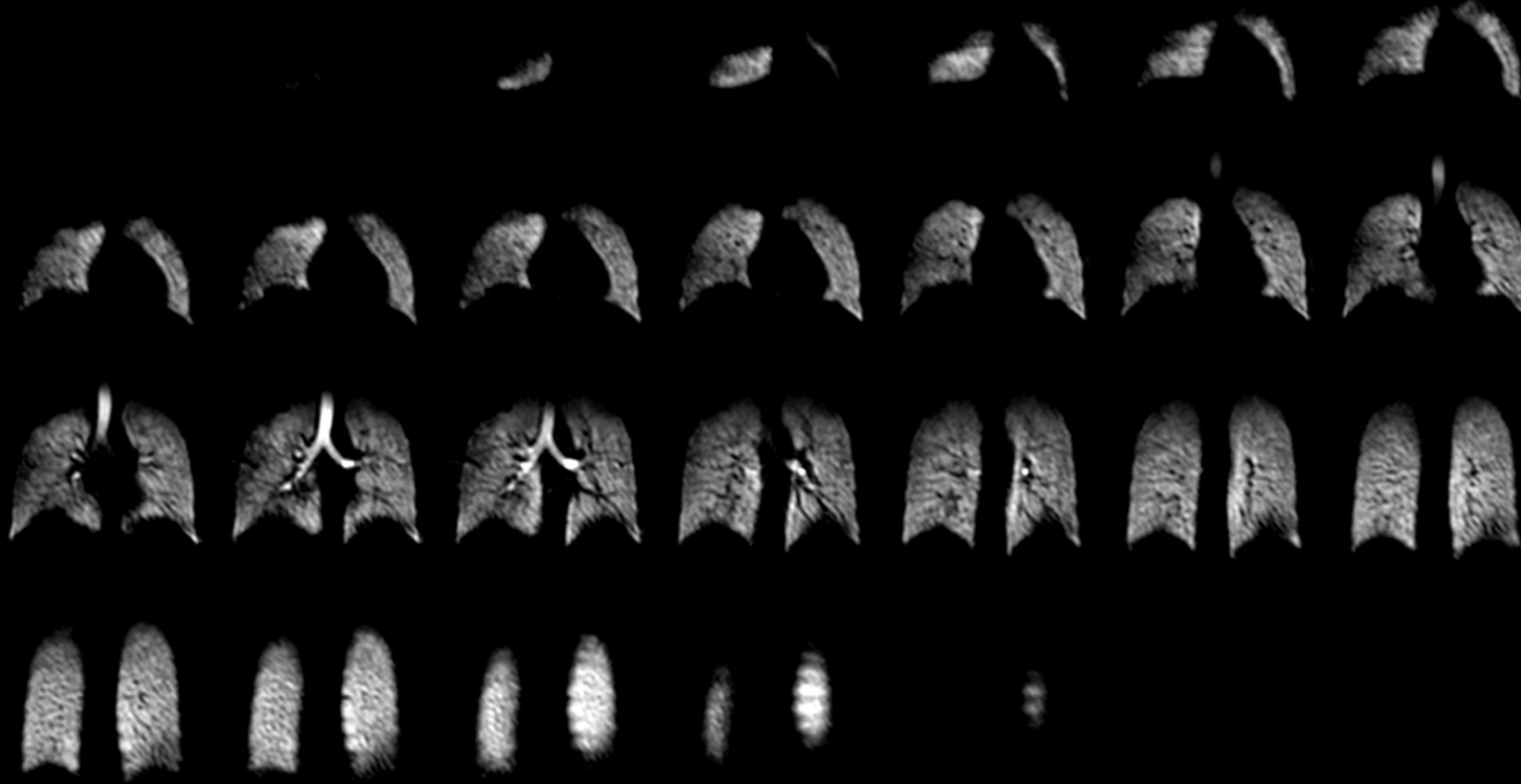
sagittal

Isotropic
resolution:
4.2 mm³



axial

3D ^{129}Xe human lung imaging with NA Xe

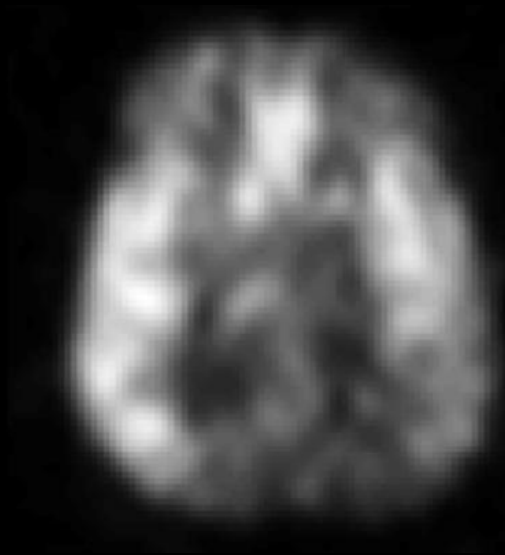


\$25/scan

1L NAXe in 20 min

Dissolved ^{129}Xe applications beyond the lungs

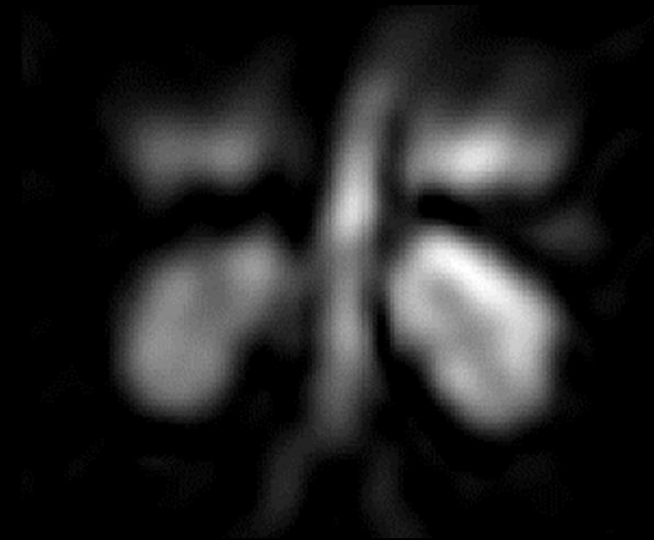
1.5 T



^{129}Xe in the brain

Rao et al., Radiology(286), 2018

3.0 T



Bottom
of lungs

Kidneys

^{129}Xe in the kidneys

Chacon-Caldera et al., MRM(83) 2019

Summary

Optimising a polariser system is a complex, multi-parameter problem

[Rb] density critical parameter for process efficiency – generally lower in practice compared with theory

Currently wide range of published exchange rate constants – more work needed

Current unknowns

Why does the SEOP cell deteriorate over time in the absence of oxidation?

Mechanism driving cell T_1 variations – orientation to B_0 field? Cell T_1 temperature dependence?