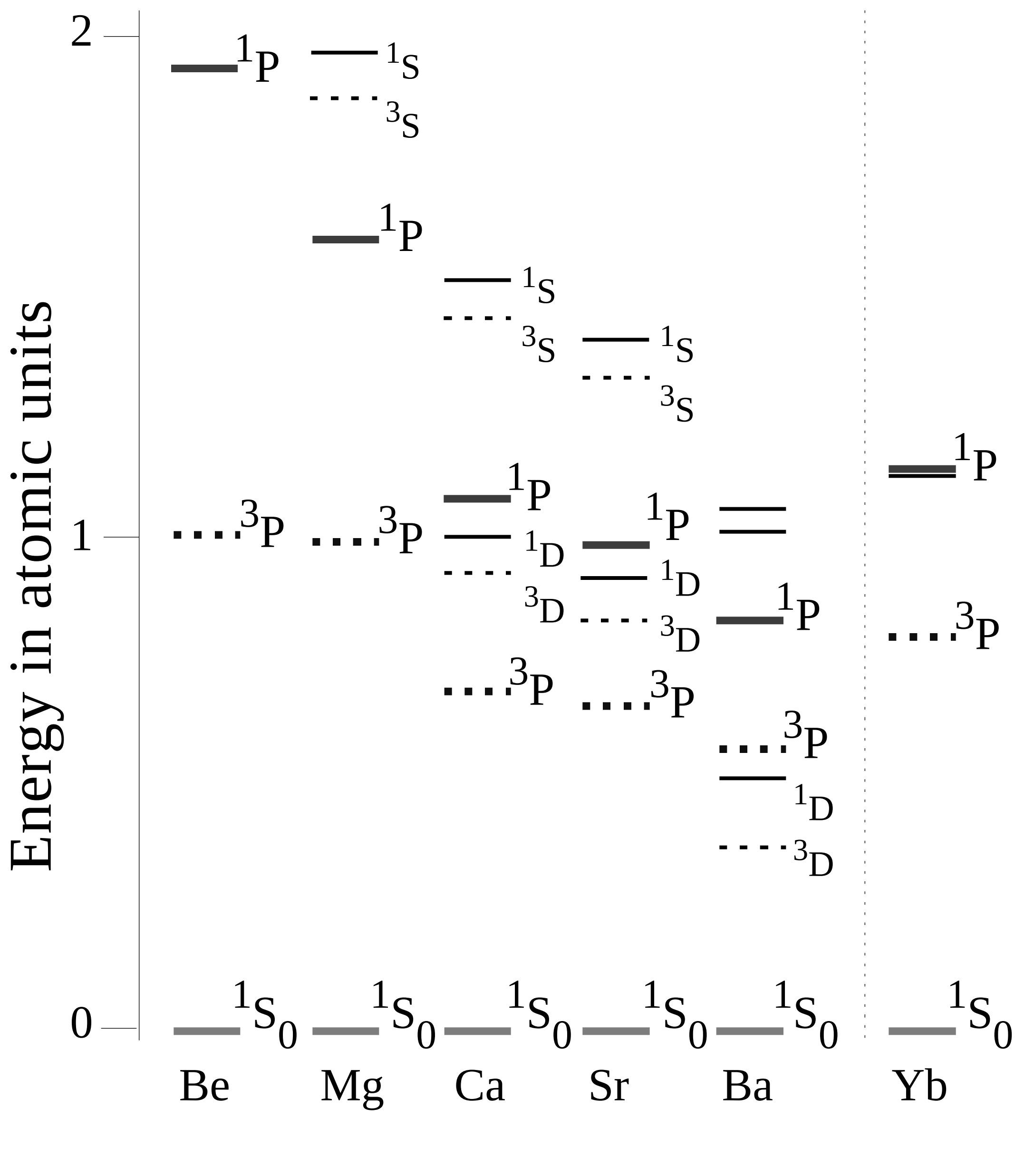
Calculations on Collisions Between Cold Alkaline Earth Atoms

Mette Machholm
National University of Singapore
Kalle-Antti Suominen
University of Turku / Helsinki Institute of Physics
Paul Julienne
National Institute for Standards and Technology

Atomic energy levels



Atomic levels

Lifetimes:

	^{24}Mg	^{40}Ca	^{88}Sr	^{138}Ba	^{174}Yb
$^{1}P_{1}$ (ns)	2.02	4.59	4.98	8.40	5.68
$^{3}P_{1}$ (ms)	2.3	0.48			
(μs)			21	1.4	0.88

Linewidths: Γ_{at} / 2 π

	Mg	Ca	Sr	Ba	Yb
$^{1}P_{1}$ (MHz)	78.8	34.7	32.0	18.9	28.0
$^{3}P_{1}$ (kHz)	0.031	0.33	7.5	120	181
d^2 (a.u.)	5.7	8.1	9.7	10.0	5.5

$V_{long\ range}(R) \sim -C_3 / R^3$ and $C_3 \sim 3\, \Gamma_{at}\, ƛ^3 / 4 = d^2$

Cooling limits

Doppler cooling limit, $\Gamma_{at}/2k_B$**:**

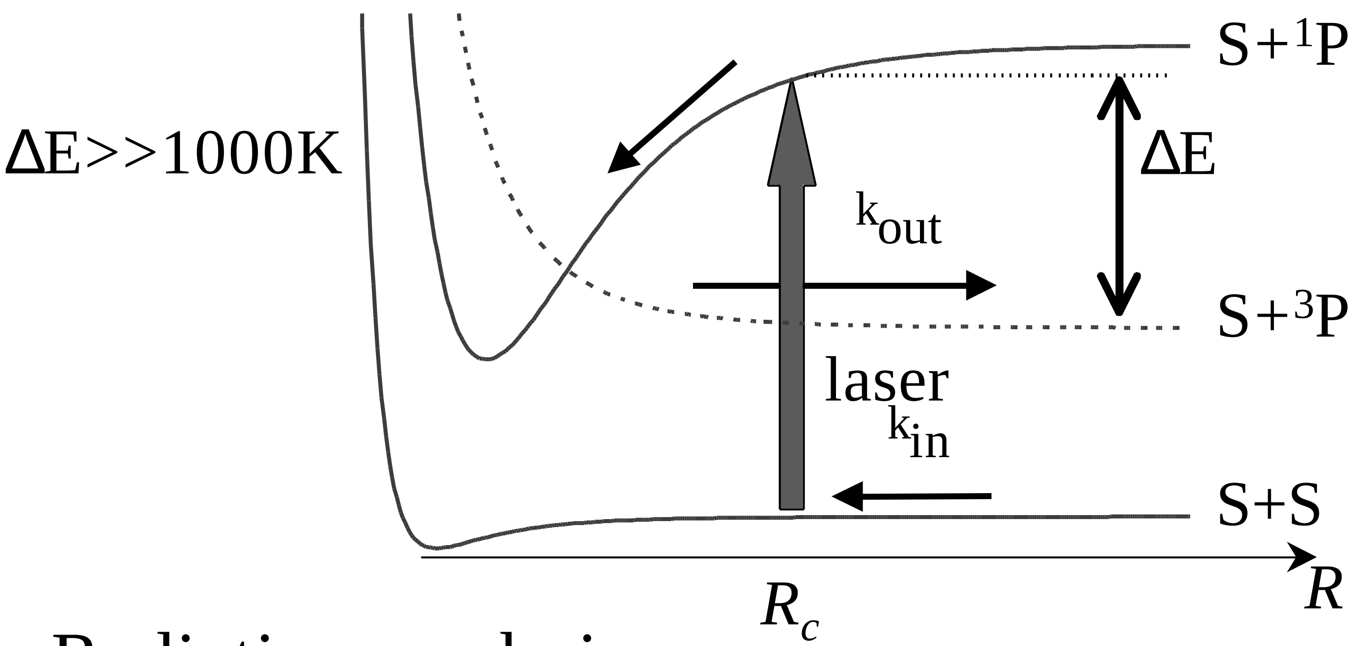
	Mg	Ca	Sr	Ba	Yb
$^1P_1$ (mK)	1.9	0.83	0.77	0.45	0.67
$^3P_1$ (nK)	**0.75**	**8.0**	**179**		
(µK)				2.8	4.4

Recoil cooling limit, $\hbar^2k^2/mk_B$**:**

	Mg	Ca	Sr	Ba	Yb
$^1P_1$ (µK)	9.8	2.7	1.0	0.45	0.69
$^3P_1$ (µK)	**3.8**	**1.1**	**0.46**	0.22	0.36

Light induced collisions

State change at small *R*



Radiative mechnisms

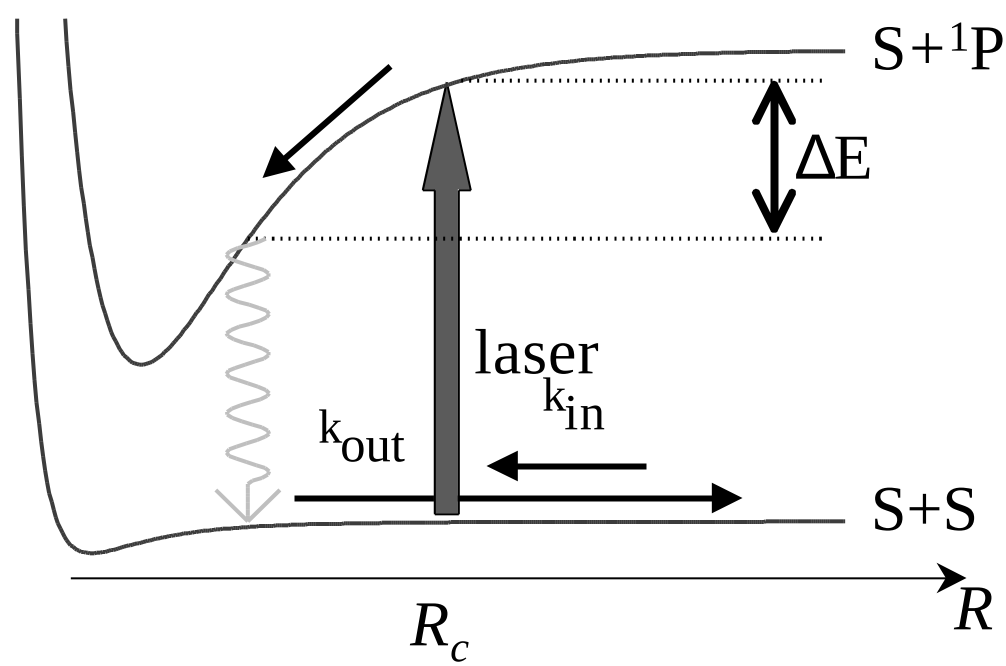
A) ΔE > 1K

Trap loss

Radiative escape

B) ΔE < 1K

Radiative heating



Long range singlet states

Relativistic retardation:

$$V_{\Sigma_u^+}(\tilde{R}) = -\frac{3\Gamma_{at}}{2\tilde{R}^3}\left[\cos(\tilde{R}) + \tilde{R}\sin(\tilde{R})\right]$$

$$V_{\Pi_g}(\tilde{R}) = -\frac{3\Gamma_{at}}{4\tilde{R}^3}\left[\cos(\tilde{R}) + \tilde{R}\sin(\tilde{R}) - \tilde{R}^2\cos(\tilde{R})\right]$$

Internuclear separation scaled: $\tilde{R} = R/\bar{\lambda}$

$\bar{\lambda} = \lambda/2\pi$

λ: the wavelength of the $^1P_1 \rightarrow {}^1S_0$ transition

Relativistic retardation important:

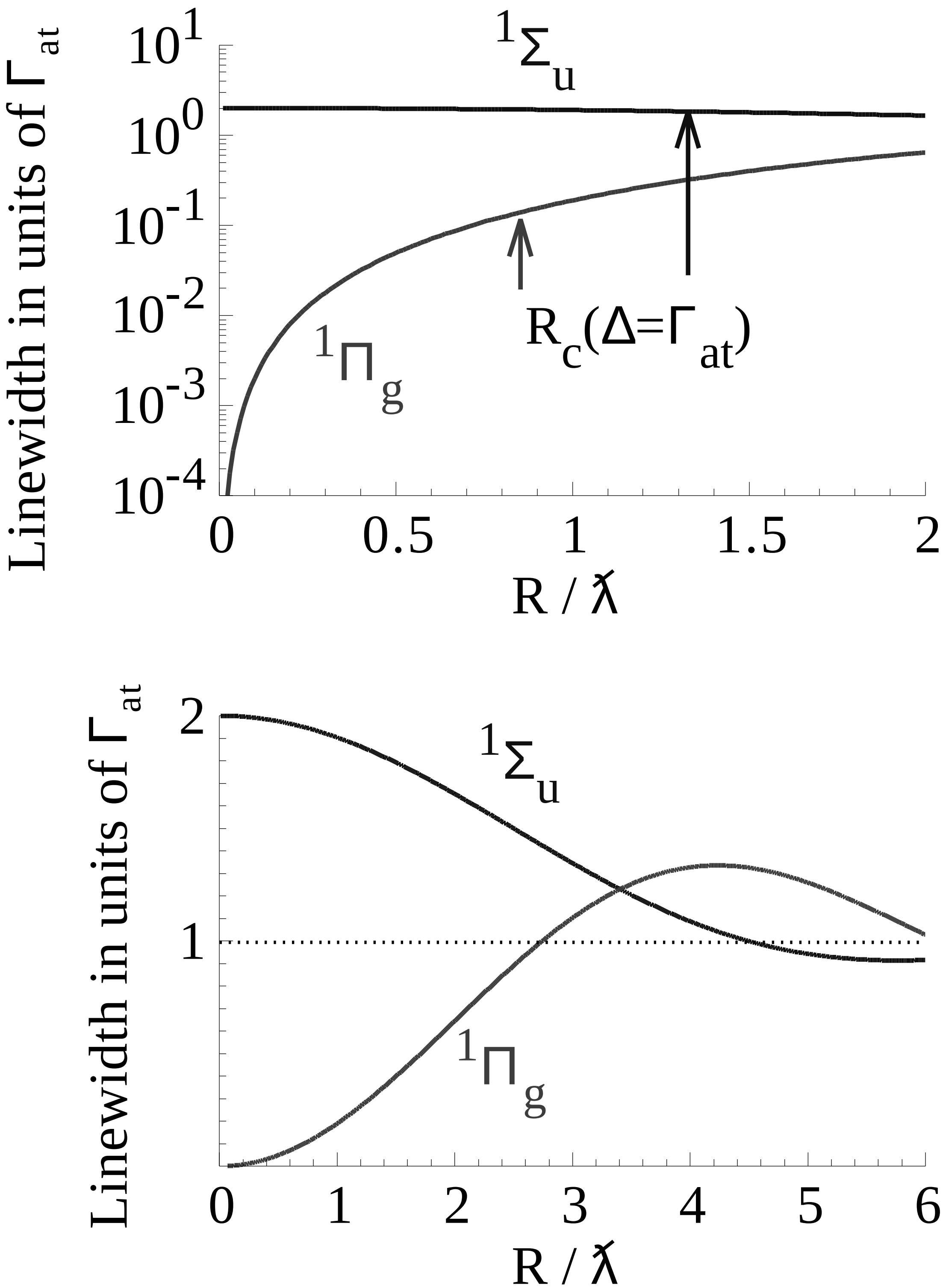
$$R > 0.35\bar{\lambda}$$

Molecular linewidths:

$$\Gamma_{\Sigma_u^+}(\tilde{R}) = \Gamma_{at}\left\{1 - \frac{3}{\tilde{R}^3}\left[\tilde{R}\cos(\tilde{R}) - \sin(\tilde{R})\right]\right\}$$

$$\Gamma_{\Pi_g}(\tilde{R}) = \Gamma_{at}\left\{1 - \frac{3}{2\tilde{R}^3}\left[\tilde{R}\cos(\tilde{R}) - \left(1 - \tilde{R}^2\right)\sin(\tilde{R})\right]\right\}$$

Retarded linewidths



Condon Point

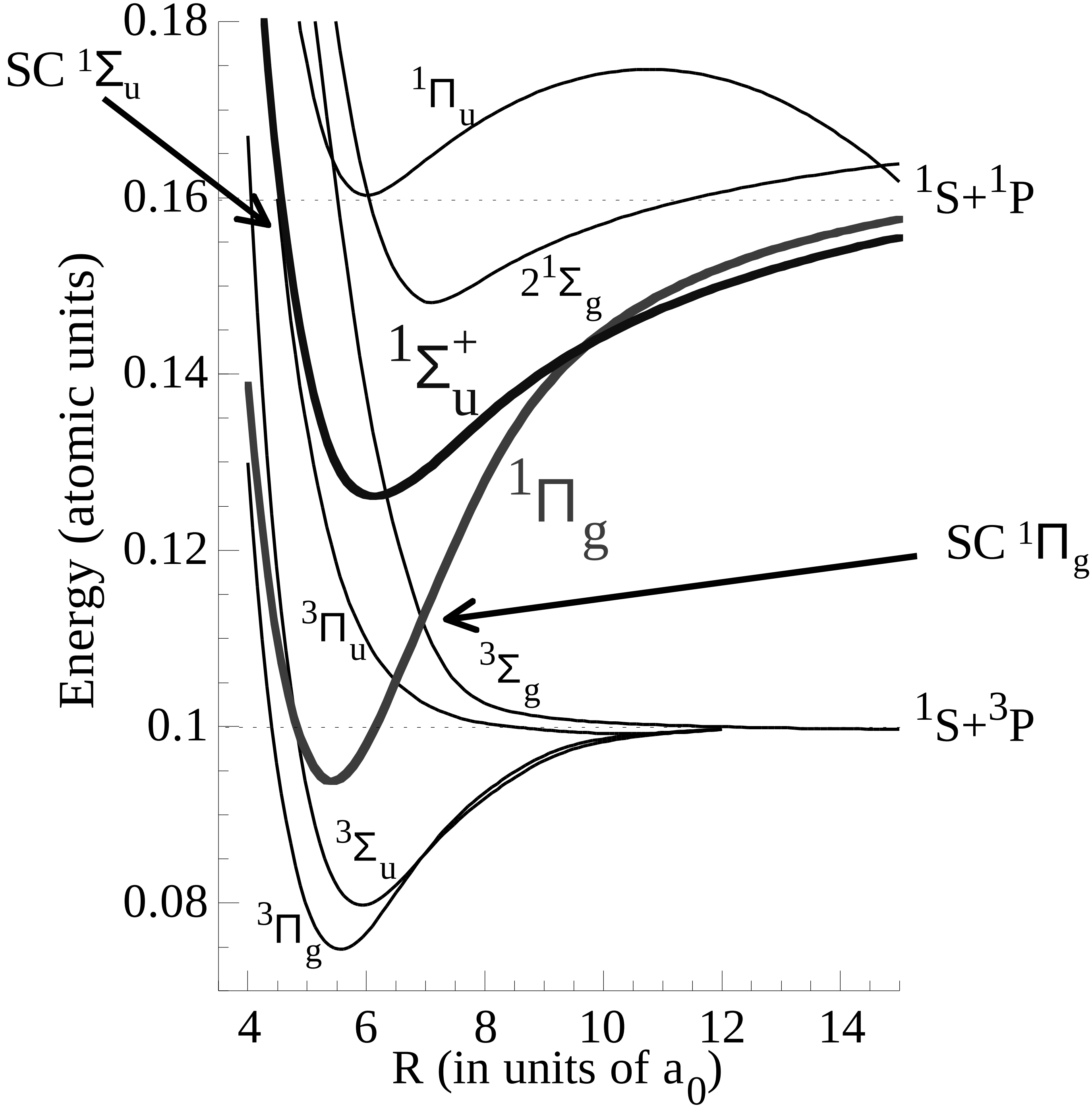
Detuning Δ in units of Γ_{at}

	$^1\Sigma_u^+$	$^1\Pi_g$
$\Delta = 1$	$R_c = 1.32\,\bar{\lambda}$	$0.85\bar{\lambda}$
$\Delta = 5$	$R_c = 0.72\,\bar{\lambda}$	$0.51\bar{\lambda}$
$\Delta = 10$	$R_c = 0.56\,\bar{\lambda}$	$0.41\bar{\lambda}$
$\Delta = 30$	$R_c = 0.38\,\bar{\lambda}$	$0.29\bar{\lambda}$

Wavelength for $^1P_1 \rightarrow {}^1S_0$

	Mg	Ca	Sr	Ba	Yb
λ (nm)	285	422	460	554	399
$\bar{\lambda}$ (a_0)	858	1271	1386	1665	1199

Mg_2 potentials



Stevens and Krauss,
JCP **67** 1977 (1977)

State change coupling

$^1\Sigma_u$	$^1\Pi_g$
$\frac{\sqrt{2}}{3}\zeta$	$\frac{1}{3}\zeta$

ζ is the FS splitting of the ^1P-states

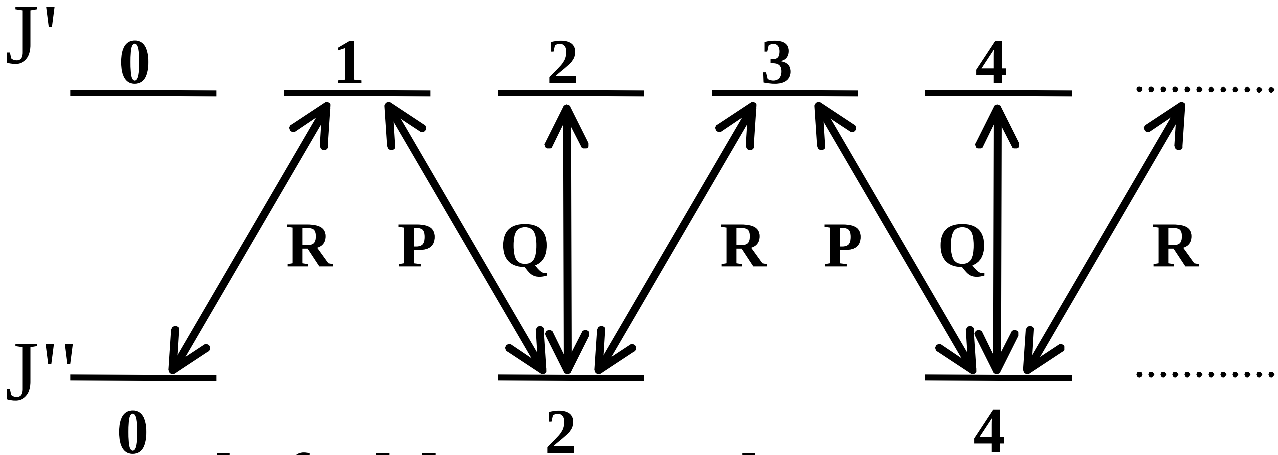
	$^3P_2$ - $^3P_0$ (in a.u.)	(in cm $^{-1}$)
Mg	$2.8 \cdot 10^{-4}$	60
Ca	$7.2 \cdot 10^{-4}$	158
Sr	$2.7 \cdot 10^{-3}$	582
Ba	$5.7 \cdot 10^{-3}$	1249
Yb	$1.1 \cdot 10^{-2}$	2414

Radiative coupling scheme

- Linearly polarized laser field
- |g〉, ground state: Σ
- |e〉, excited states:

Σ-state: **P** & **R** branches

Π-state: **P**, **Q** & **R** branches



- Weak field approach

  Independent sum over ground state partial waves and branches

  (no partial wave "ladder climbing")

Complex potential approach

Solve the time-independent Schrödinger equation for 3 coupled states:

|g , |e ($^1\Sigma_u$/$^1\Pi_g$) and a probe state (SC/RE)

Kinetic term

Molecular potentials

Laser coupling of |g> and |e> states

Coupling at small R for SC

Collision energy

Complex decay term

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2} + U(R) + V(R) + H_{SO} - \varepsilon - i\hbar\Gamma(R)\right)\Psi(R) = 0$$

Find S-matrix elements for transfer between the |g> and SC state, > 2500 grid points in *R*

Trap loss rates

Loss rate for 1 energy ε and detuning Δ

$$\mathbf{K}(\Delta,\varepsilon) = \left.\frac{\mathbf{k_B T}}{\mathbf{hQ_T}}\right|_{\mathbf{k_B T}=\varepsilon} \sum_{l_{\mathbf{even}}} (2l+1) \sum_{\mathbf{B}=\mathbf{P},\mathbf{Q},\mathbf{R}} \left|\mathbf{S_{gp}}(\varepsilon,\Delta,l,\mathbf{B})\right|^2$$

Energy averaged for 1 temperature:

$$\mathbf{K}(\Delta,\mathbf{T}) = \frac{\mathbf{k_B T}}{\mathbf{hQ_T}} \int_0^\infty \frac{\mathbf{d}\varepsilon}{\mathbf{k_B T}} \exp(-\varepsilon/\mathbf{k_B T})$$

$$\times \sum_{l_{\mathbf{even}}} (2l+1) \sum_{\mathbf{B}=\mathbf{P},\mathbf{Q},\mathbf{R}} \left|\mathbf{S_{gp}}(\varepsilon,\Delta,l,\mathbf{B})\right|^2$$

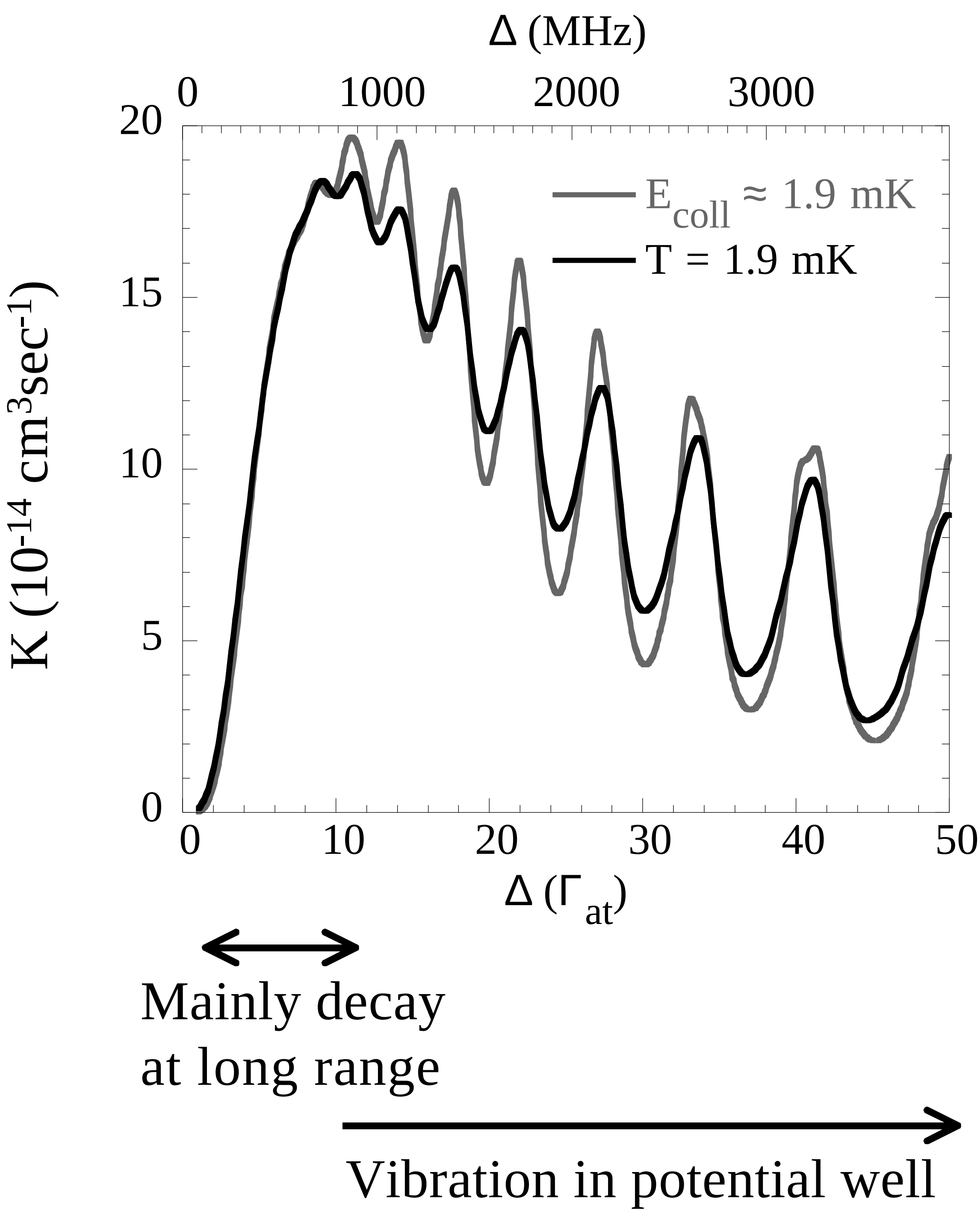
200 - 600 ε -values

< 80 partial waves, 2-3 branches

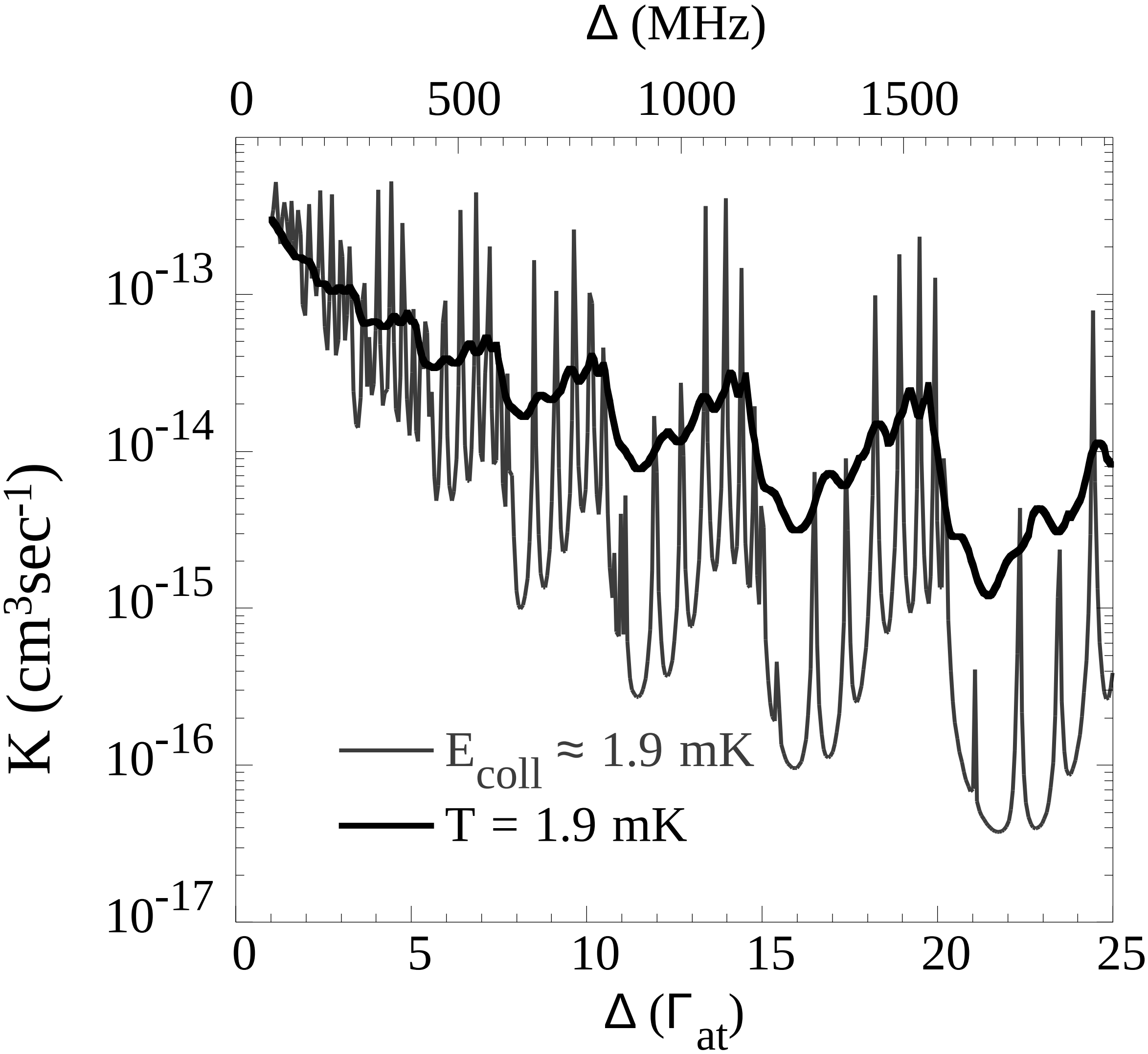
Up to 140 000 S_{gp} per Δ

$^1\Pi_g$ dense grid in ε and Δ

Mg, $T=T_{doppler}$
State Change $^1\Sigma_u^+$



Mg, T=$T_{doppler}$
State Change $^1\Pi_g$



If excitation to $^1\Pi_g$ then little decay
high trap loss for small detunings

Calculation method RE

- Probe and excited states cross at 1K (trap depth set to T = 0.5 K)
- Probe state depends on partial wave and detuning
- Factorization of trap loss probability: $|S_{pg}|^2 = P_{g\text{-}e} \cdot J_e \cdot P_{e\text{-}p}$

$P_{RE} = P_{g\text{-}e} \cdot J_e \cdot P_{decay}$

$P_{decay} = (1 - e^{-a})$ $\quad$ $a = 2\int_{R_{1K}}^{R_{in}} dR \frac{\Gamma(R)}{v(R)}$

$P_{e\text{-}p}$ depend on l, ε and Δ

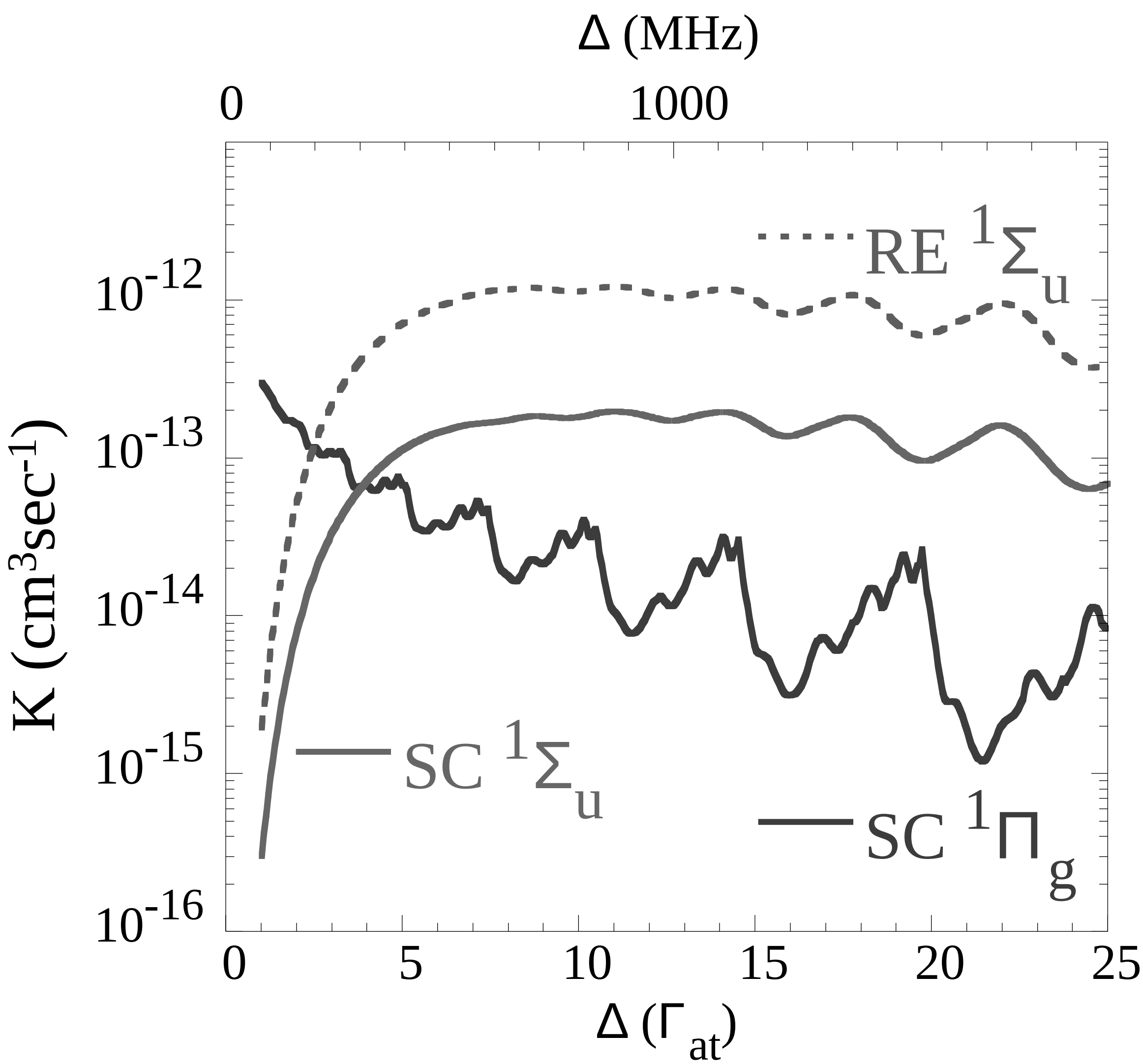
Use:

No complex term $\quad J_e = 1$

Saturate excitation $\quad P_{g\text{-}e} \approx 1$

Mg, T=$T_{doppler}$

State Change & Radiative Escape



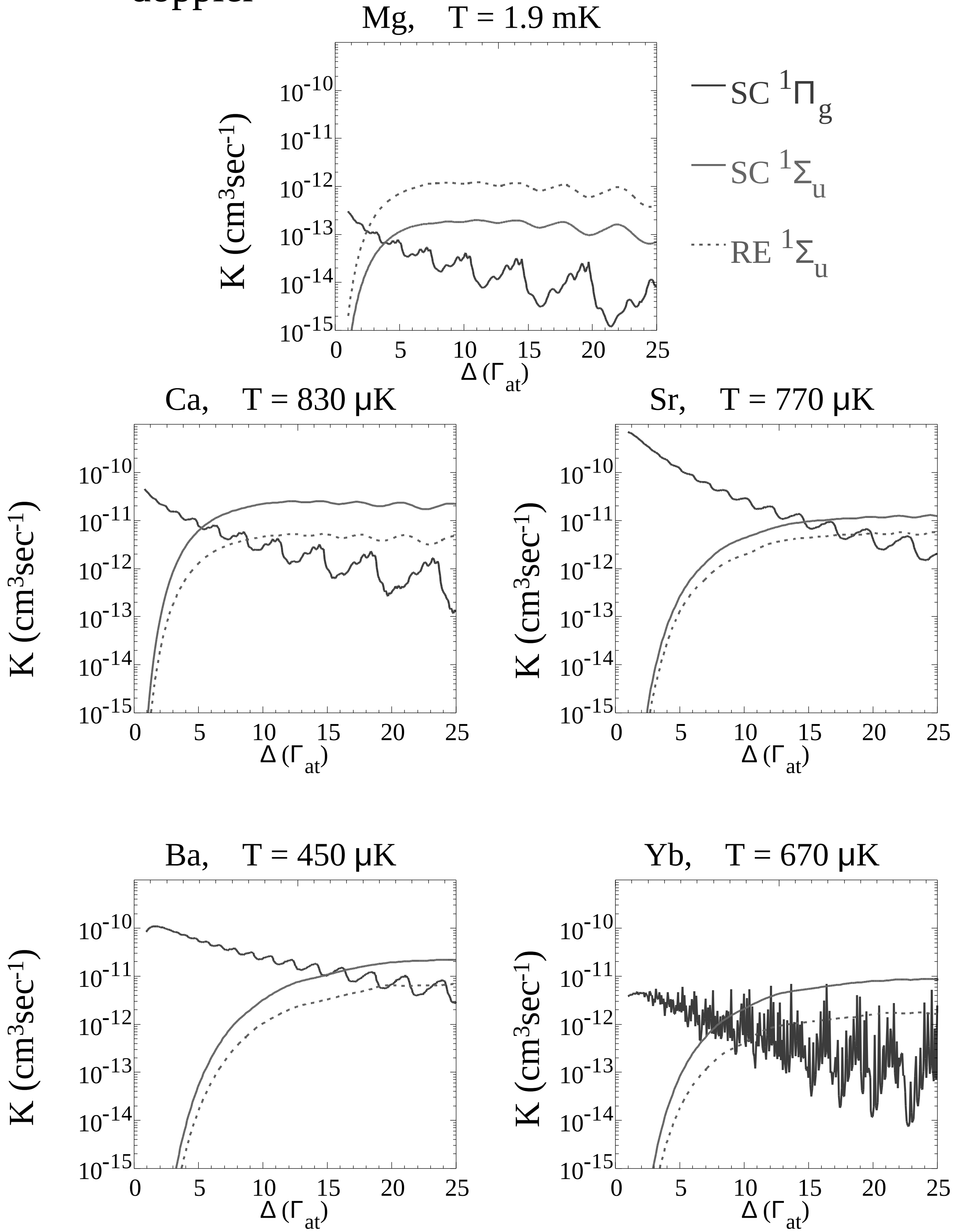
Relative magnitude of SC Σ and RE Σ determined by the short range SC coupling

Ca, Sr, Ba and Yb

- 3 state models
- Exact long range potentials
- One SC channel to account for complex short range structure
- SC coupling scaled by the splitting of the ^3P states
- SC transition probabilities:

	$^1\Sigma_u$	$^1\Pi_g$
Mg	1.8-2.3 %	0.01-1%
Ca	40-47 %	0.2-40 %
Sr	29-33 %	2-100 %
Ba	32-36 %	0.3-40 %
Yb	61-68 %	0.3-10 %

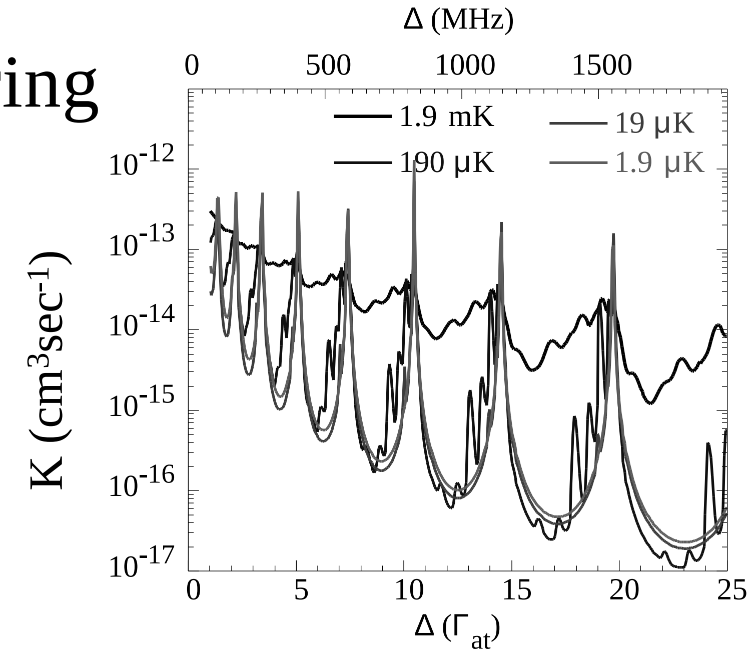
$T = T_{doppler}$


Mg, T = 1.9 mK
Ca, T = 830 μK
Sr, T = 770 μK
Ba, T = 450 μK
Yb, T = 670 μK
K (cm^{3}sec^{-1})
Δ (Γ$_{at}$)
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
0
5
10
15
20
25
SC $^1\Pi_g$
SC $^1\Sigma_u$
RE $^1\Sigma_u$

Lower temperature: $^1\Pi_g$

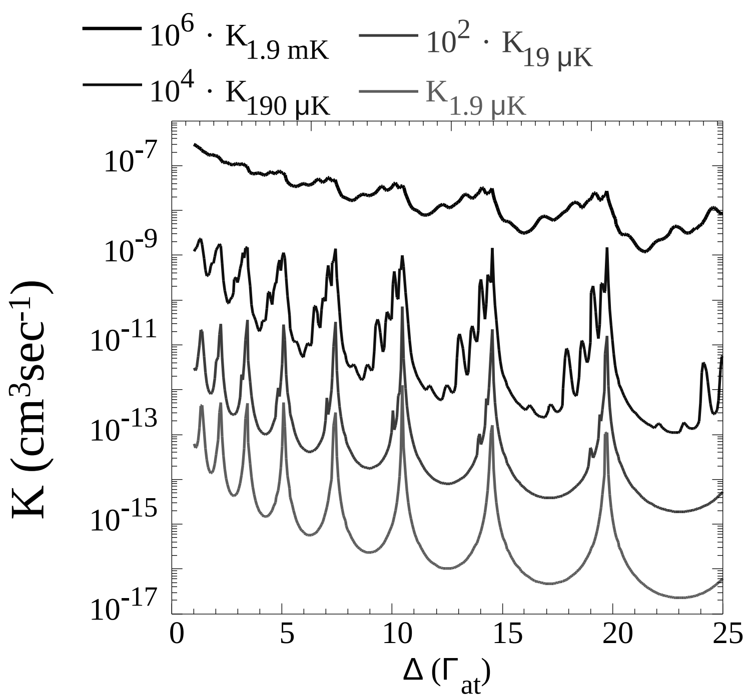
Mg: $T_{doppler}$ = 1.9 mK T_{recoil} = 1.9 μK

Pure s-wave scattering close to the T_{recoil}



At $T_{doppler}$:

vibrational structure



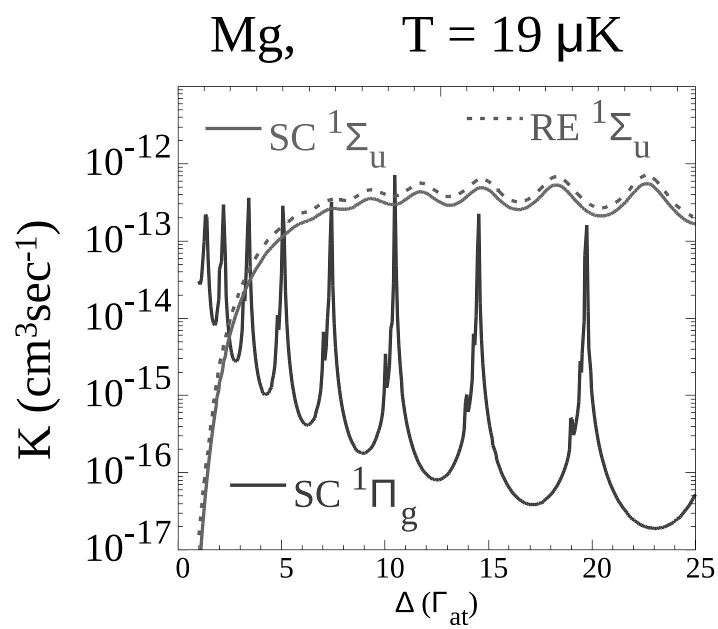
At 0.1·$T_{doppler}$:

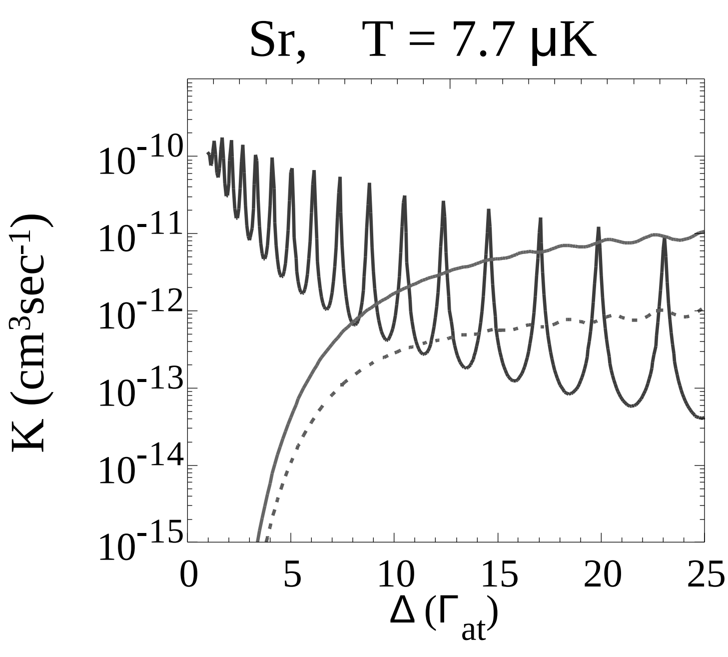
ro-vibrational structure

Lower temperature: $^1\Sigma_u$

Relative magnitude of RE and SC

K_{SC} / K_{RE} increases as T decreases





Experimental values, Mg

- Madsen & Thomsen:

  Mg: $6*10^{-10}$ cm^3/s

  $\Delta = \Gamma_{at}$

  $I = 400$ mW/cm^2

  $T > T_{Doppler}$

- Theory

  $3*10^{-13}$ cm^3/s

  $I=1$ mW/cm^2

  $T=T_{doppler}$

  Assume linear Scaling with I

  => 10^{-10} cm^3/s

Experimental values, Sr

- Gallagher et al:

  Sr: $4.5*10^{-10}$ cm^3/s (7%/25%)

  $\Delta = 1.75\ \Gamma_{at}$

  I = 60 mW/cm^2

  $T \sim 4\ T_{Doppler}$

- Theory

  $5*10^{-10}$ cm^3/s

  I=1 mW/cm^2

  $T=T_{doppler}$

  Assume linear Scaling with I

  => $3*10^{-8}$ cm^3/s

  Saturation of $^1\Pi_g$ excitation?

  SC probability << unity? Most likely

  Difference due to temperature?