Molecular MOT OBE Simulations in *Julia*

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Preliminary I: OBEs

Reminder: What are OBEs?

Optical Bloch Equations:

master equation for time evolution of quantum state under light-matter interaction Hamiltonian.

$$\frac{\partial \hat{\rho}}{\partial t} = \frac{1}{i\hbar}\left[\hat{H}, \hat{\rho}\right] - \left[\sum_{p=-1}^{1} \frac{\Gamma}{2}(\hat{S}_p^{\dagger}\hat{S}_p\hat{\rho} - \hat{S}_p\rho\hat{S}_p^{\dagger} + h.c)\right]$$

Coupled set of ODEs, one equation per component of ρ with constraints of Hermiticity and conservation of probability

$$\hat{S}_p \propto \sum_{F,J,m,F'} \left(\langle F', J', m_F' | T_p^{(1)}(\mathbf{d}) | F, J, M_F\rangle\right) |F, J, m_F\rangle\langle F', J', m' = m + p|$$

Quantum “jump” operator

$$\hat{H} = \sum_{F,J,m_F} E_{F,J}|F, J, m_F\rangle\langle F, J, m_F| + \sum_{F',J',m_F'} E_{F',J'}|F', J', m_F'\rangle\langle F', J', m_F'|$$
$$+ \left(-\hat{\mathbf{d}}\cdot\hat{\mathbf{E}}(\boldsymbol{r}, t) - \hat{\boldsymbol{\mu}}\cdot\hat{\mathbf{B}}(\boldsymbol{r}, t)\right).$$

Atom-light interaction Hamiltonian in hyperfine energy basis

Reminder: What are OBEs?

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Coherent evolution from H_{int}

Spontaneous decay from excited states (Lindblad “quantum jump” operator)

Reminder: What are OBEs?

Intuitive derivation in 2-level system:

$|\psi\rangle = \begin{pmatrix} c_g \\ c_e \end{pmatrix}$. $\hat{\rho} = |\psi\rangle\langle\psi|$ for pure state. So $\hat{\rho} = \begin{pmatrix} |c_g|^2 & c_g c_e^* \\ c_g^* c_e & |c_e|^2 \end{pmatrix}$.

Schrödinger Eqn: $i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$, $-i\hbar \frac{d\langle\psi|}{dt} = \langle\psi|\hat{H}$.

$$i\hbar \frac{d\hat{\rho}}{dt} = i\hbar \frac{d}{dt}\left(|\psi\rangle\langle\psi|\right) = \left(i\hbar \frac{d|\psi\rangle}{dt}\right)\langle\psi| + |\psi\rangle\left(i\hbar \frac{d\langle\psi|}{dt}\right)$$

$$= \hat{H}|\psi\rangle\langle\psi| + \cancel{i\hbar}\,|\psi\rangle \cdot \frac{1}{\cancel{i\hbar}}\langle\psi|\hat{H} \quad \therefore \quad \boxed{\dot{\hat{\rho}} = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}].}$$

Reminder: What are OBEs?

Intuitive derivation in 2-level system:

Add in effects from spontaneous decay: $\dot{\rho}_{ee} = -\Gamma \rho_{ee}$ $\dot{\rho}_{gg} = \Gamma \rho_{ee}$ $\dot{\rho}_{eg} = -\frac{\Gamma}{2} \rho_{eg}$

Full OBE for 2-level system: $\dot{\hat{\rho}} = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}] + \begin{pmatrix} \Gamma \rho_{ee} & -\frac{\Gamma}{2}\rho_{ge} \\ -\frac{\Gamma}{2}\rho_{eg} & -\Gamma \rho_{ee} \end{pmatrix}$

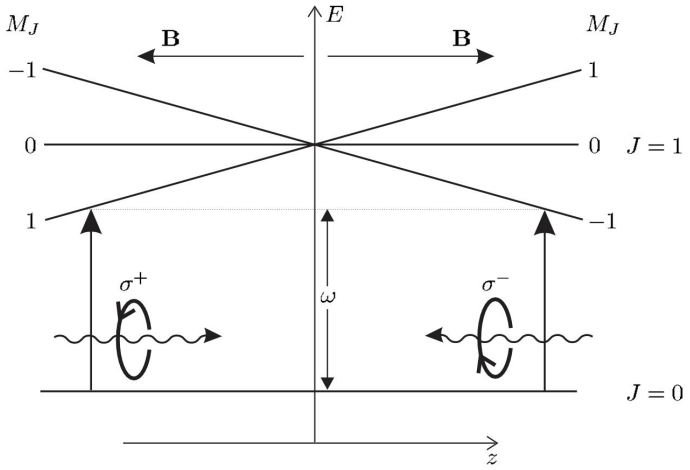
$\hat{H} = \hbar \begin{pmatrix} \Delta/2 & \Omega/2 \\ \Omega/2 & -\Delta/2 \end{pmatrix}$ in RWA and rotating frame

For further details/insights, see: Lukin AMO notes, Metcalf, DeMille, etc…

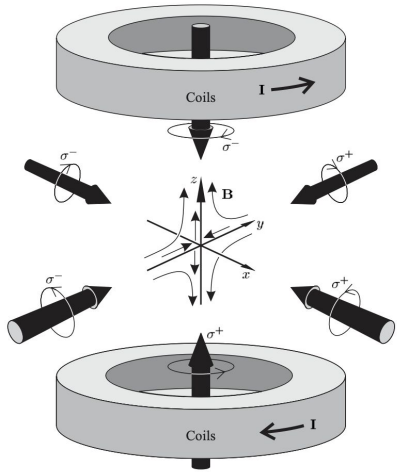
Bottom line: in code, OBEs time-evolve quantum state of atoms/molecules as they interact w/MOT light and trapping B-field.

Preliminary II:
MOT Physics and Setup in Code

Reminder: How do MOTs work?



Simplest case: J = 0 → J' = 1



Experimental setup for MOT

- **Doppler cooling** from optical molasses - **velocity-dependent damping force**
- **Zeeman splitting** creates imbalance in radiation pressure - **spatially-dependent restoring force**

$$F_{scat} \sim p_\gamma \underbrace{R_{scat}}_{\Gamma \rho_{ee}} = \hbar k \frac{\Gamma}{2} \frac{s}{1 + s + \frac{4\tilde{\Delta}^2}{\Gamma^2}}$$

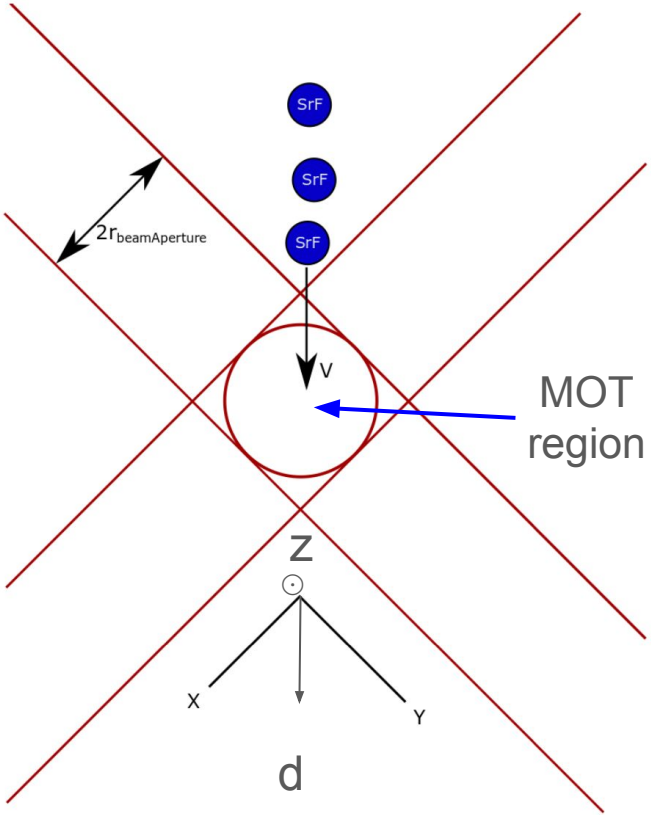
$\tilde{\Delta}$ is function of Δ, kv, $\frac{\partial B}{\partial z} z$ in MOT.

(1-D) force on atom/molecule in MOT:

$$F_{tot} \sim -Kz - \alpha v, \quad K = K\left(\Delta/\Gamma, \frac{\partial B}{\partial z}\right), \quad \alpha = \alpha\left(\Delta/\Gamma\right).$$

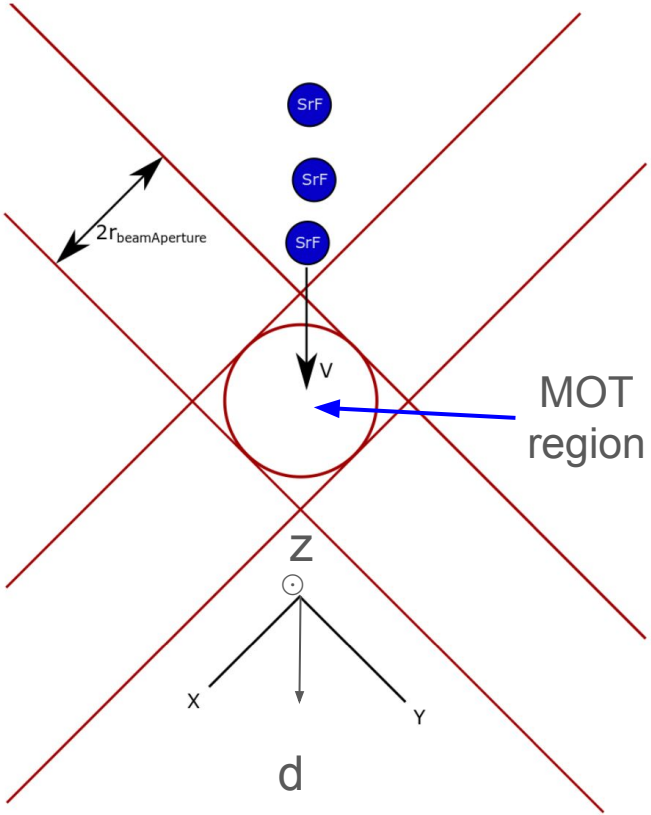
Model MOT like damped harmonic oscillator

Setup of MOT in OBE Simulator Code



- **MOT laser beams in x,y,z directions.**
- Define **d ≡ (x+y)/√2** as **molecule beam axis**. Molecules enter from -d direction.
- Define **origin** as **center of MOT.**
- Lasers and B-field are 3-D but **only compute forces along d-direction (1-D).**
- Code accounts for finite laser beam size using $r_{beamAperture}$ and defines MOT capture region as intersection between laser beams.

Setup of MOT in OBE Simulator Code



Initial Parameters:

- **Initialize molecule at (d_{trial}, v_{trial})** where d_{trial} and v_{trial} are taken from pre-determined sets of d and v in code.
- **Molecule starts at random position in cube** (x'=0,z'=0, d=d_{trial}) to (x'=λ, z'=λ, d=d_{trial}+λ) - primes denote rotated xy-plane. **Accounts for λ-scale polarization/intensity gradients.**
- **NumTrials** → # random positions chosen from cube per value of (d_{trial}, v_{trial}).

Units and Periodicity:

- Express **freq. in units of Γ**, **vel. in units of k/Γ**, **pos. in units of 1/k**
- Discreteness of simulation → **round freqs** to nearest integer multiple of **"discretized freq unit" $\omega_r = \Gamma/N$**, N integer.
- **ρ periodic with $\tau = 2\pi/\omega_r$** in steady-state (time-dependent H). **Time-evolve ρ until initial transients dissipate**; evolve for one more period and calculate dynamical variables of interest.

Preliminary III:
Calculating MOT Dynamics in Code

Calculating Force in QM

Start from Heisenberg equation of motion for an operator:

$$\hat{F}(t) = \frac{d\hat{p}(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{p}(t)\right]. \qquad \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}).$$

Momentum is generator of translations.

$$\left[\hat{H}, \hat{p}(t)\right] = \left[V(\hat{x}), \hat{p}(t)\right]. \qquad \hat{p} = \frac{\hbar}{i}\nabla \Rightarrow \left[V(\hat{x}), \hat{p}\right] = i\hbar\frac{\partial V(\hat{x})}{\partial \hat{x}}$$

$$\therefore \hat{F}(t) = -\frac{\partial V(\hat{x})}{\partial \hat{x}} \sim \hat{F}(t) = -\frac{\partial H_{int}}{\partial r}.$$

To compute force in code, compute spatial derivative of H_{int}.

Averaging over Ensemble and Hamiltonian Periodicity

- Quantum mechanics valid for an ensemble (for which probabilities have meaning).
- **"Ensemble average" force over density matrix** (all possible quantum states for atom/molecule):

$$\left\langle \hat{F}(\vec{r},\vec{v},t) \right\rangle = Tr\left[\hat{\rho}(t)\,\hat{F}(\vec{r},\vec{v},t)\right] = Tr\left[\hat{\rho}(t)\left(-\frac{\partial \hat{H}_{int}}{\partial r}\right)\right].$$

Crux of OBE code: time-evolve ρ, compute ensemble-averaged spatial derivative of H_{int}.

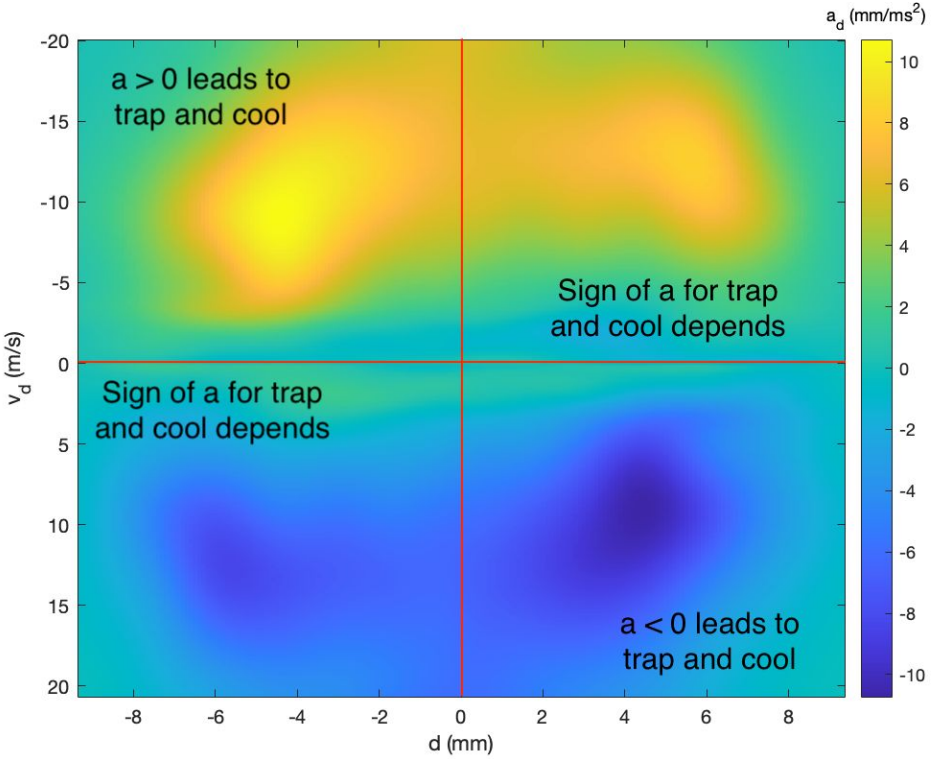
- **Time-average the ensemble average over 1 period** of Hamiltonian periodicity:

$$\left\langle \hat{F}(\vec{r},\vec{v}) \right\rangle = \frac{1}{\tau}\int_{t_{tr}}^{t_{tr}+\tau} \left\langle \hat{F}(\vec{r},\vec{v},t) \right\rangle dt$$

t_{tr} is time it takes for initial transients to dissipate

- Finally, **average force above over all random positions in initial λ-sized cube** to account for λ-scale fluctuations in polarization/intensity.

Heat Map of $a(d, v_d)$



- Obtain acceleration $a(d, v_d)$ by dividing force by molecule mass.
- "Heat map" of $a(d, v_d)$ obtained by 2-D spline interpolation between initial $\{d, v_d\}$ points.

Heat map of $a(d, v_d)$ contains all information about MOT dynamics.

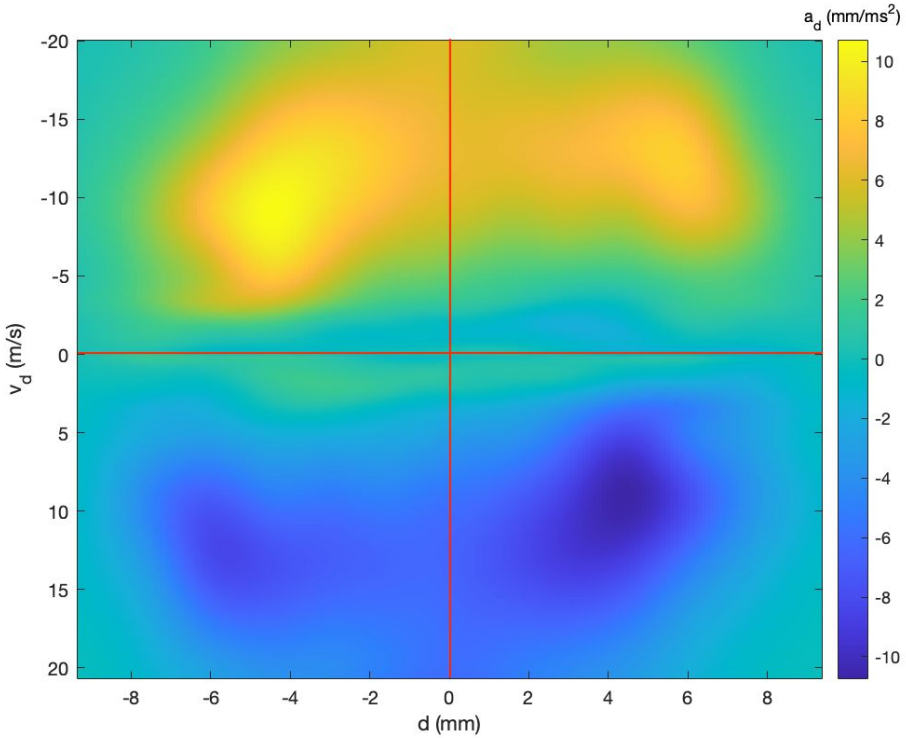
MOT equation of motion:

$$\ddot{d} = -\alpha\dot{d} - kd, \quad \alpha, k > 0.$$

Sign of a for $d>0$, $v_d<0$ or vice versa depends on strength of damping α and restoring k

Given initial (d, v_d) values, we can map out trajectory of MOT via straightforward time integration.

Obtaining a(d) and a(v_d) curves



Obtain **more intuition about MOT dynamics by "collapsing" heat map along one axis**. This means taking a "1-D average" along that axis.

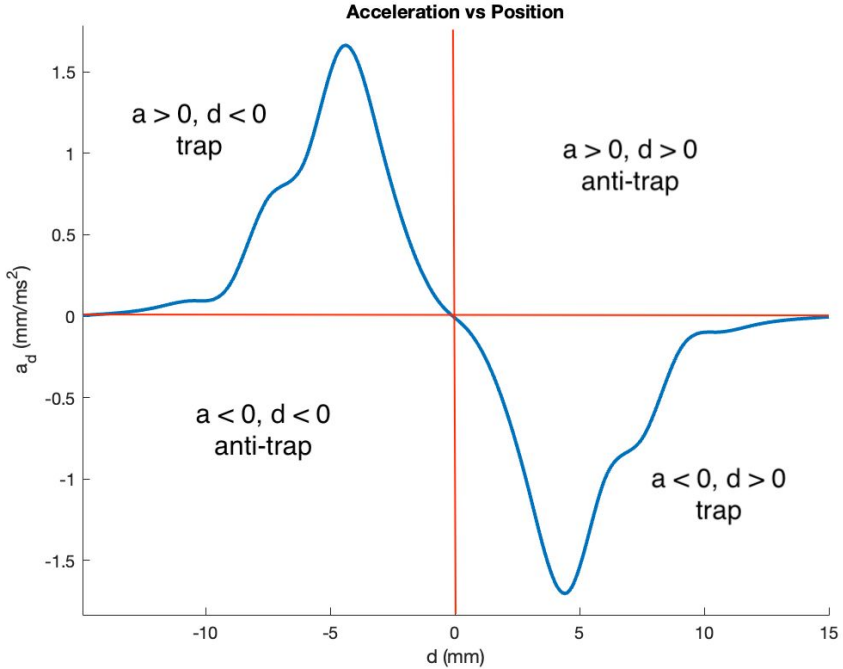
Collapse horizontal axis (d) → a(v_d) plot

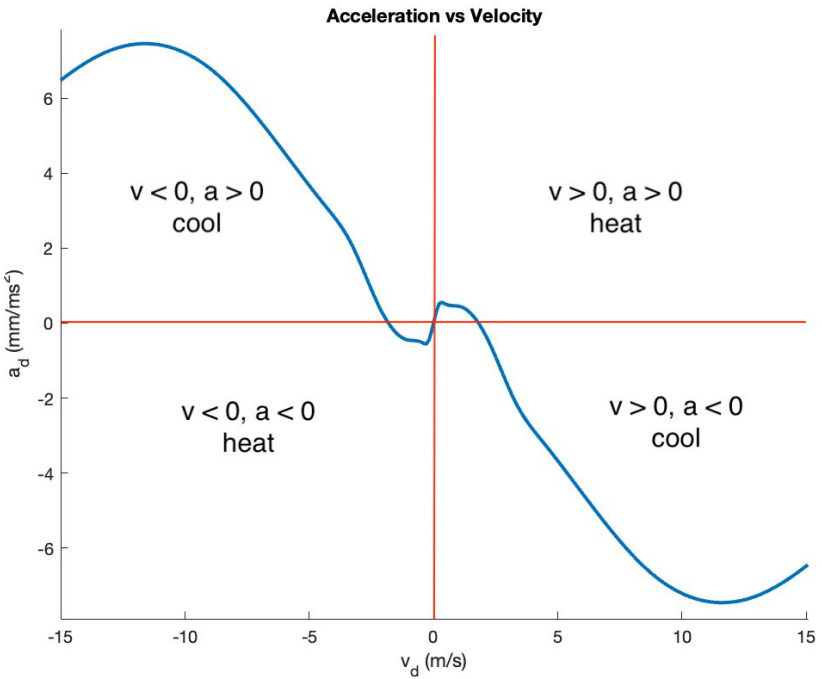
$$a_d(v_d) = \frac{1}{2d_{max}} \int_{-d_{max}}^{d_{max}} a_d(d, v_d)\, d(d)$$

Collapse vertical axis (v_d) → a(d) plot

$$a_d(d) = \frac{1}{2v_{d,max}} \int_{-v_{d,max}}^{v_{d,max}} a_d(d, v_d)\, dv_d$$

Example a(d) and a(v_d) plots





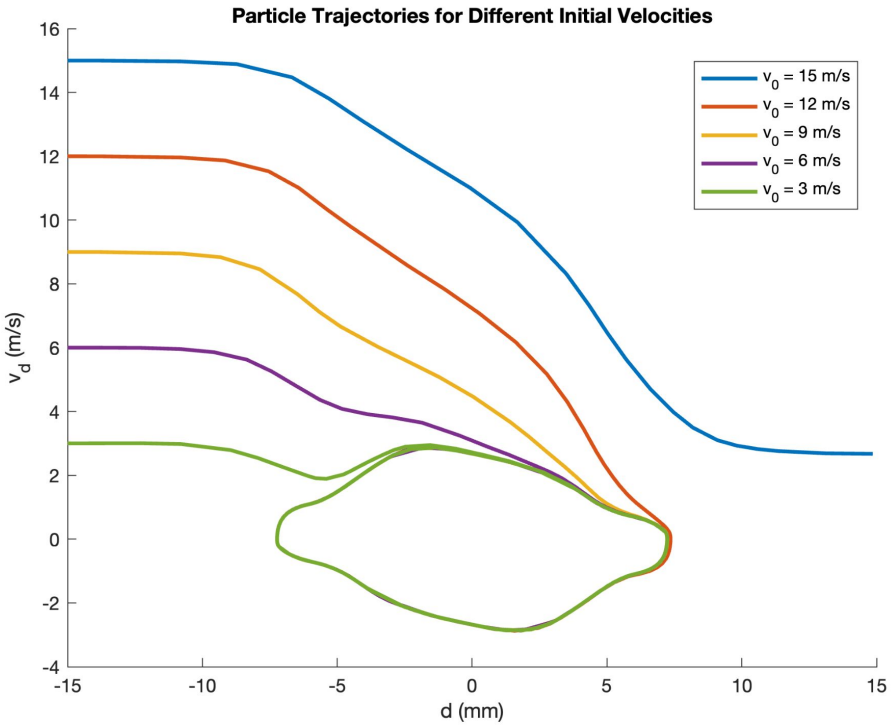
Damped SHO is odd in d, v_d individually

Evidence of sub-Doppler heating at close range
(as expected for Type-II transition in laser-cooled molecules)

Computing Capture Velocity of MOT

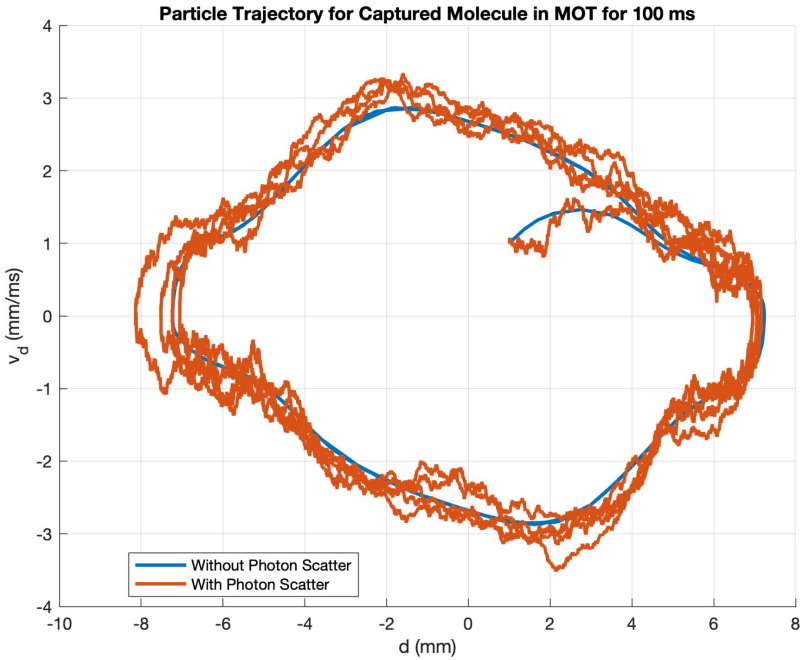
- **Begin molecule at initial (d_{max}, v_d) value** (where **d_{max} < 0 is maximum d used in trials** and $v_d > 0$, i.e. molecule heads from source towards MOT capture region).
- **Compute trajectory using heat map a(d, v_d)** via numerical time integration.
- **If, within 20 ms, molecule is turned around before reaching $|d_{max}|$, then it counts as being captured.**
- **Increment initial v_d until above is no longer true. The maximum v_d before this occurs is deemed the capture velocity.**
- For captured molecules, add additional time evolution of 100 ms after “capture” to show molecule remains trapped in MOT. **Also can account for random photon scatter in MOT from spontaneous emission and show MOT remains robust.**

Phase Space Plots of Capture into MOT



- Left, shows phase space plot of MOT capture for all v_d < 15 m/s.
- **Captured molecules in MOT enter "merry-go-round"** in phase-space
- **Large spatial extent** (-5 mm < d < 5 mm) and **velocity extent** (-3 m/s < v_d < 3 m/s) of capture MOT likely due to **Type-II-induced sub-Doppler heating**
- Capture MOT can be made smaller by compression, blueMOT, etc…

Phase Space Plot of Trajectory in Capture MOT



- Trapped molecule starts at (d = 1 mm, v_d = 1 mm/ms).
- **Trapped molecule remains in equilibrium in MOT** with stable oscillations in velocity from -3 mm/ms < v_d < 3 mm/ms and position from -8 mm < d < 8 mm.
- Phase space plot includes trajectory with (red) and without (blue) photon scatter.
- Even **accounting for randomized photon scatter, capture MOT is robust to trapping.**
- Define **rms width σ** of capture MOT as **$\sigma = \sqrt{\langle d^2 \rangle}$** and **temperature T** as **$T = m\langle v_d^2 \rangle / k_B$** (equipartition thm).
- For **example plot** shown:
  - **Capture MOT has σ ≈ 5 mm and T ≈ 33 mK**.

Typical Parameters Used in Simulations

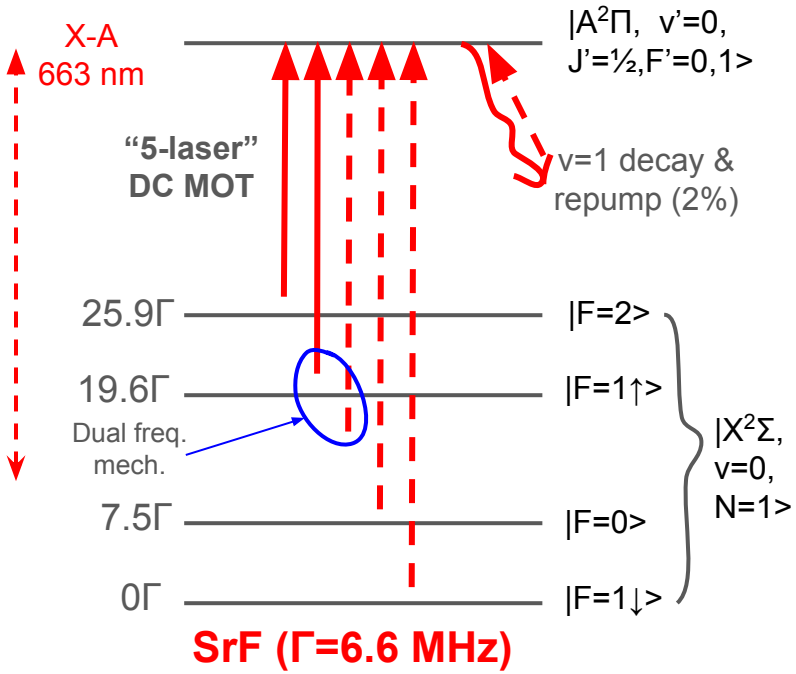
Example a(d,v_d) heat map, MOT phase space plots, etc. shown previously were calculated using following "typical" simulation parameters:

- **Molecule = SrF. Monochromatic X-A MOT.**
  - Note: **original version of "testCode.jl"** in "MinimumWorkingExampleMOTSimulator" is **hard-coded for $^2\Sigma$ alkaline-earth monofluoride molecules**, amenable to laser cooling.
- **MOT B-field gradient** (code uses radial gradient): **8 G/cm**.
  - Axial B-field gradient is 2x radial due to divergence-free B-field in free space.
- **MOT laser beam waist** (code uses $1/e^2$ beam radius): **7 mm.**
- **Set of {d, v_d} values** used in simulation:
  - $d \in \{0.5, 1.5, 3.0, 4.5, 6.0, 7.5, 9.0, 10.5, 12, 13.5, 15\}$ mm.
  - $v_d \in \{-5, -4, -3, -2, -1, -0.75, -0.5, -0.25, -0.1, -0.05, 0.05, 0.1, 0.25, 0.5, 0.75, 1, 2, 3, 4, 5\}$ Γ/k. Here, for **SrF X-A transition, Γ/k = 4.4 m/s**.
- **Number of trials per (d, v_d) value: 50** (accounting for random fluctuations in λ-scale cube).
- laserVariables.dat in 20240907_1943 run contains further details on MOT laser freq detunings, saturation intensity, and polarization.
- **No vibrational repump** was used for the example simulation. Presence of v=1 vibrational repump introduces 12 extra ground states to couple to; reduces scattering rate and effectiveness of MOT.

Results:
Molecular MOTs (SrF and CaF)

Molecular MOT Level Scheme

- To-date, most **diatomic molecular MOTs** follow **alkaline-earth-halide motif** (SrF, CaF, BaF)
  - $^2\Sigma$-$^2\Pi$ electronic structure for optical quasi-cycling (unpaired electron spin)
- **Focus on SrF and CaF X-A MOTs** in the following (to **replicate results from TKL *NJP* (2023) paper**).

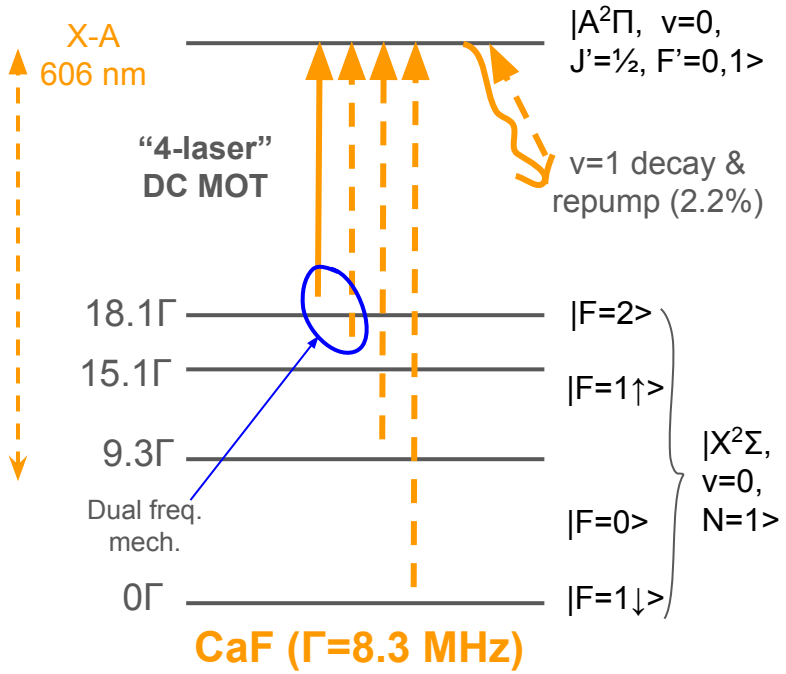


Laser polarization

σ^+

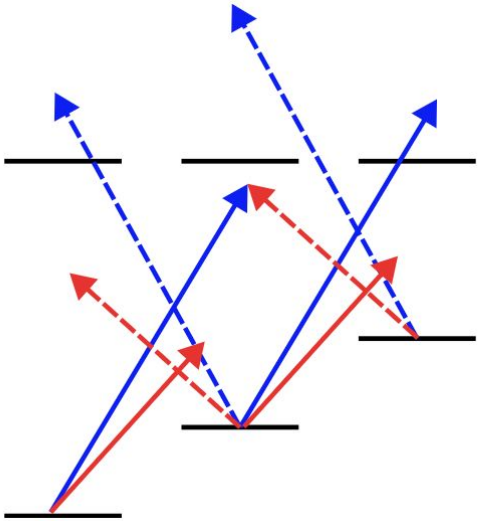
σ^-

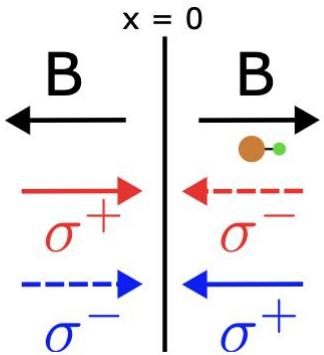
MOT laser detuning, saturation, polarization all tunable in simulation



Dual-frequency mechanism for DC Molecular MOTs

All molecular MOTs require driving Type-II ($J_g > J_e$, where J denotes total angular momentum) optical cycling transitions for rotational closure.





Dual-freq. mech. illustrated for $J_g > J_e$ and $g_g >> g_e$, as is case for laser-cooled molecules.

- **Dual-frequency mechanism: simultaneously send light of opposite detuning and polarization** along beam path.
- **$m_F = \pm 1$ ground states preferentially absorb optical cycling light**
- **$m_F = 0$ ground state has equal likelihood of absorbing any optical cycling light**
- Gives strong net MOT scattering force to molecule, no dark states in principle
- Expect much stronger and more robust DC MOT with this scheme compared to no dual-frequency mechanism (where only 1 g.s. m_F level preferentially absorbs light)

Trials explored for Molecular MOT Simulations

Cases below did NOT incorporating vibrational branching/repumping.

1. Vary the MOT laser beam waist
2. Vary the MOT B-field gradient
3. Vary the MOT laser beam saturation parameter
4. Sanity check: is dual-frequency mechanism in polarization needed for MOT?
5. Sanity check: does all-blue detuning of laser frequencies destroy capture MOT?
6. Compare SrF MOT standard configuration to CaF MOT standard configuration

No vibrational branching speeds up performance by reducing # of quantum states to incorporate in simulation.

Finally, do two “real cases” incorporating vibrational branching/repumping on v=1.

1. Standard SrF configuration (as per TKL *NJP* 2023 paper).
2. Standard CaF configuration (as per TKL *NJP* 2023 paper).

Compare SrF MOT vs CaF MOT performance (with v=1 vibrational branching - more realistic).

“Canonical” Parameters for Molecular MOT Simulations

50 trials run for each unique (d, v_d) to avg out fluctuations during random initialization of d in λ-sized cube.
Default molecule used is SrF. Default no vibrational branching to speed up code (less states).

- Initial molecule positions and velocities sampled:
  - d ∈ {0.5, 1.5, 3.0, 4.5, 6.0, 7.5, 9.0, 10.5, 12, 13.5, 15} mm.
  - v_d ∈ {-5, -4, -3, -2, -1, -0.75, -0.5, -0.25, -0.1, -0.05, 0.05, 0.1, 0.25, 0.5, 0.75, 1, 2, 3, 4, 5} Γ/k.
  - For SrF, Γ/k = 4.4 m/s. For CaF, Γ/k = 5.0 m/s.
- MOT beam waist size: 7 mm (radius)
- MOT B-field gradient: 8 G/cm (radial)
- MOT beam saturation parameters (5-laser MOT):
  - [F=1↓, F=0, F=1↑b, F=2, F=1↑r] = [10, 20, 10, 31.3, 8.7]
- MOT beam frequencies (5-laser MOT): freq/energy referenced to F=1↓ energy level (0Γ)
  - [F=1↓, F=0, F=1↑b, F=2, F=1↑r] = [-1.1Γ, -9.8Γ, -18.6Γ, -26.8Γ, -20.8Γ]
- MOT beam polarizations (5-laser MOT):
  - [F=1↓, F=0, F=1↑b, F=2, F=1↑r] = [1, 1, 1, -1, -1] (here, ±1 indicates $\sigma^{\mp}$ polarization).
  - Dual-frequency on F=1↑ since F=1↑b and F=1↑r have opposite polarizations.

“Canonical” Parameters for Molecular MOT Simulations

For CaF simulations: MOT beam waist size and B-field gradient same.

- MOT beam saturation parameters (4-laser MOT):
  - [F=1↓, F=0, F=1↑, F=2] = [20, 20, 20, 20]
- MOT beam frequencies (4-laser MOT): freq/energy referenced to F=1↓ energy level (0Γ)
  - [F=1↓, F=0, F=1↑, F=2] = [-1.4Γ, -10.7Γ, -16.1Γ, -19.5Γ]
- MOT beam polarizations (4-laser MOT):
  - [F=1↓, F=0, F=1↑, F=2] = [1, 1, 1, -1] (here, ±1 indicates $\sigma^{\mp}$ polarization).
  - Dual-frequency on F=2 since F=1↑ and F=2 have opposite polarizations.

For SrF and CaF comparison with vibrational branching to v=1, used parameters from TKL *NJP* (2023) paper (see Table 1, pg. 8 for SrF and Table D1, pg. 33 for CaF).

Note: when one variable is varied, all other variables are held at the “canonical” value unless otherwise specified.

Molecular MOT Simulation Data File Index

List of data files for all trials follows. Canonical trial for SrF (no vib. branching) is 20240910_2054.

1. Vary MOT beam waist:
   a. w = 5 mm: 20240911_0927
   b. w = 9 mm: 20240911_0050
2. Vary B-field gradient:
   a. b = 5 G/cm: 20240911_1333
   b. b = 15 G/cm: 20240911_1804
3. Vary MOT beam saturation parameters:
   a. Half of canonical saturation parameters: 20240912_1128
   b. Tenth of canonical saturation parameters: 20240913_2356
4. Check if dual frequency is necessary for MOT: 20240913_1025 (make all lasers same polarization)
5. Check if all blue-detuning destroys MOT: 20240913_1443
6. Compare to canonical CaF parameters (no vib. branching): 20240913_1906

With vibrational branching to v=1:

1. SrF: 20240911_2215.
2. CaF: 20240912_2021.

SrF MOT performance vs laser beam waist size

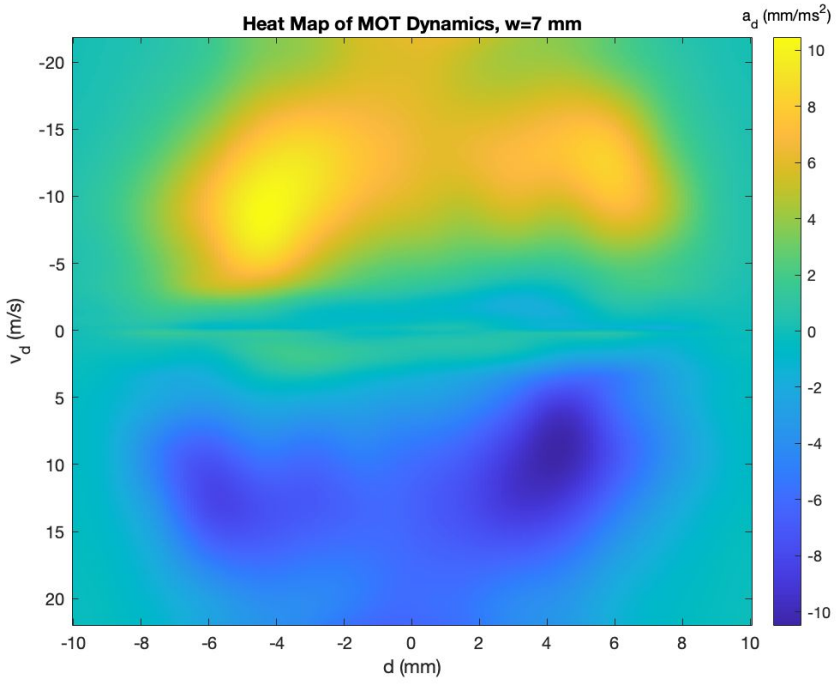
Waist radius (mm)	MOT rms size (mm)	MOT temp (mK)	MOT capture velocity (m/s)
5	3.8	39.8	11.2
7	4.8	36.8	14.1
9	5.9	40.9	16.1

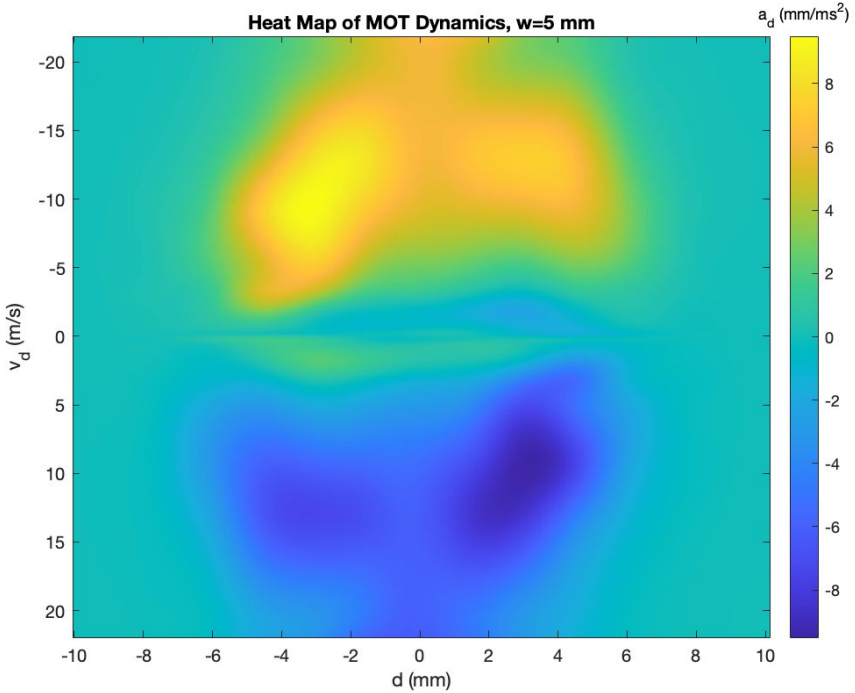
Trend. **As laser beam waist is increased:**

- **MOT size increases**
- **MOT temperature stays roughly the same**
- **MOT capture velocity increases**

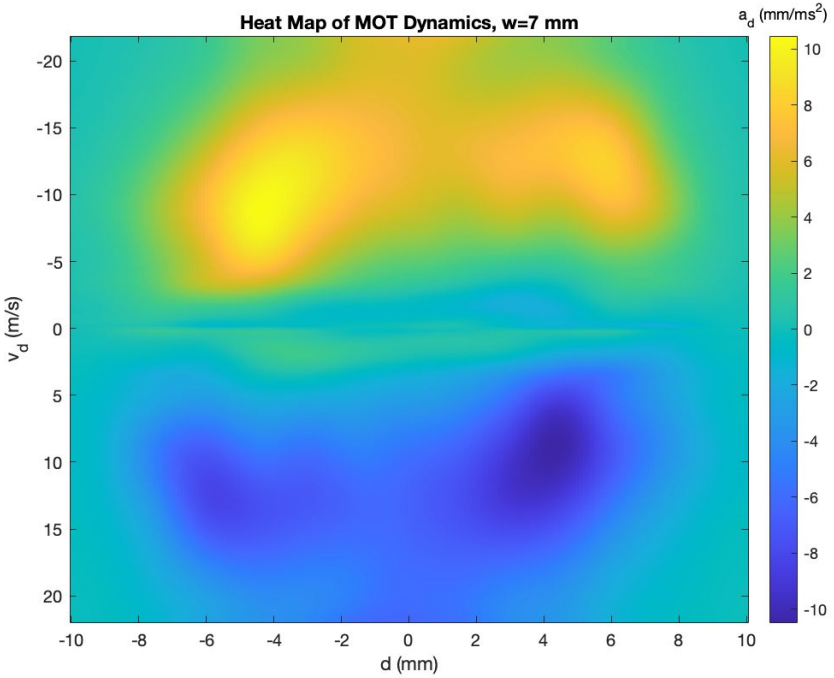
Reasoning: as **MOT beam waist is increased**, the **capture volume and laser power delivered is larger**. This enables **larger MOTs and higher capture velocities**.

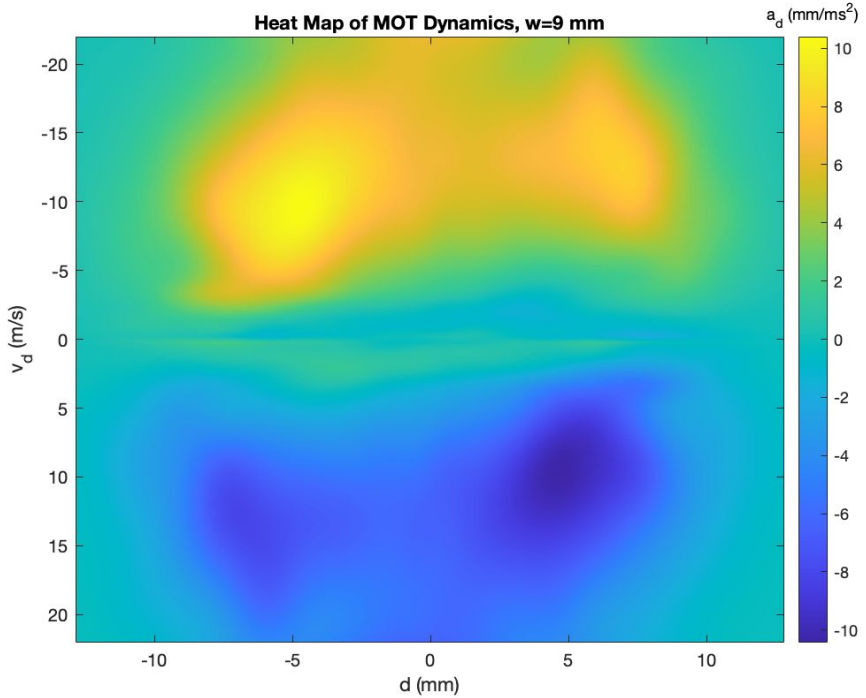
SrF MOT performance vs laser beam waist size





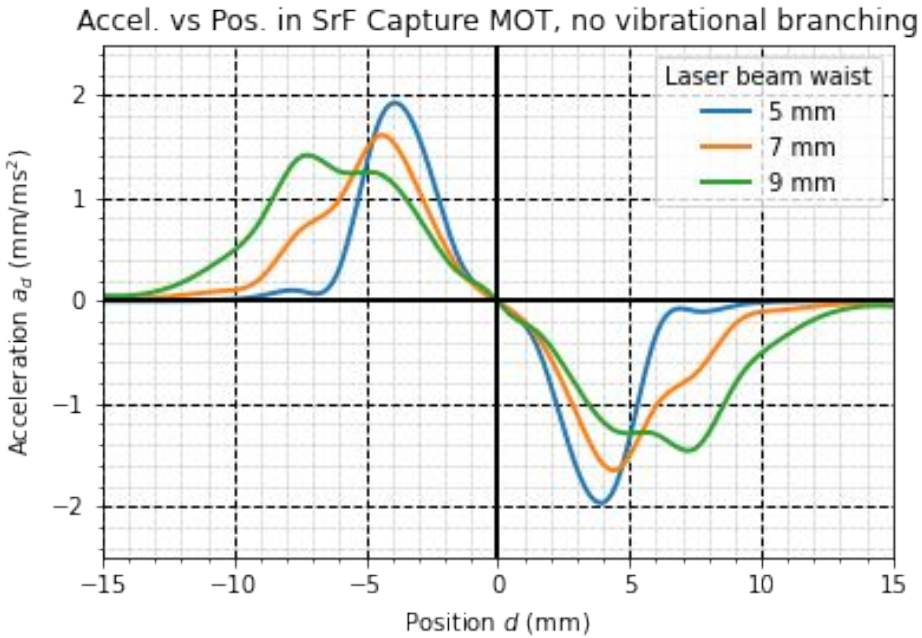
SrF MOT performance vs laser beam waist size

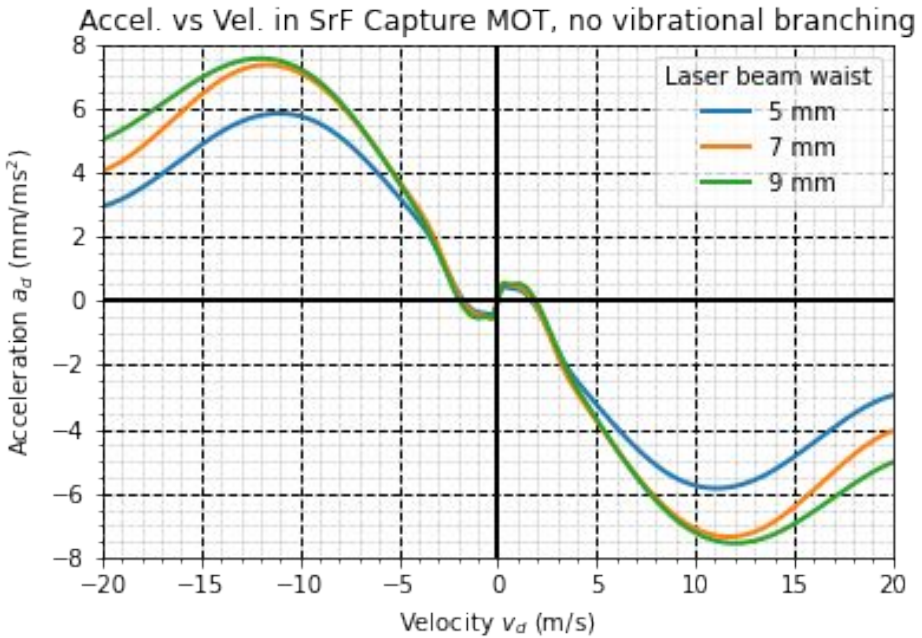




Heat map shows “larger” effective (d, v_d) region for w=9 mm vs. w=5 mm.

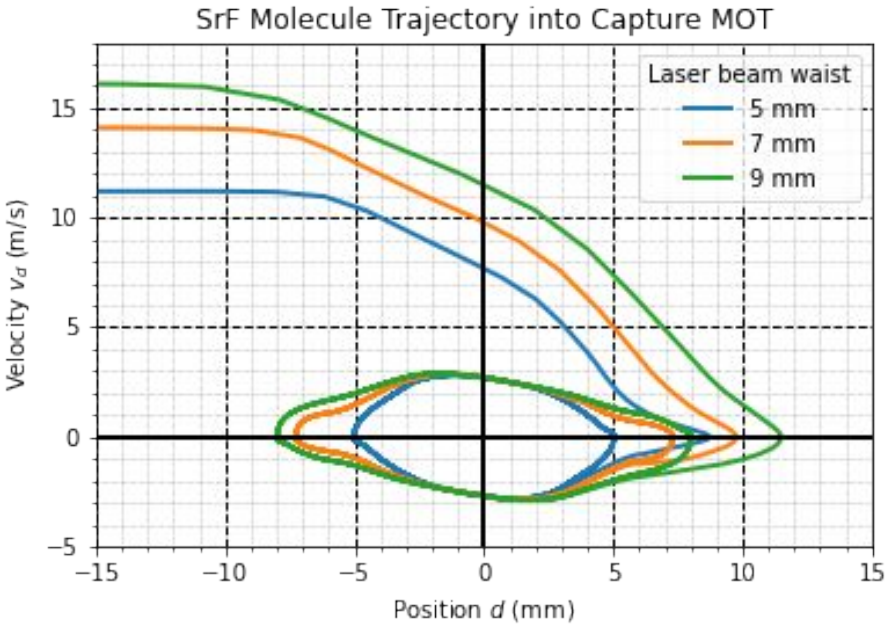
SrF MOT performance vs laser beam waist size

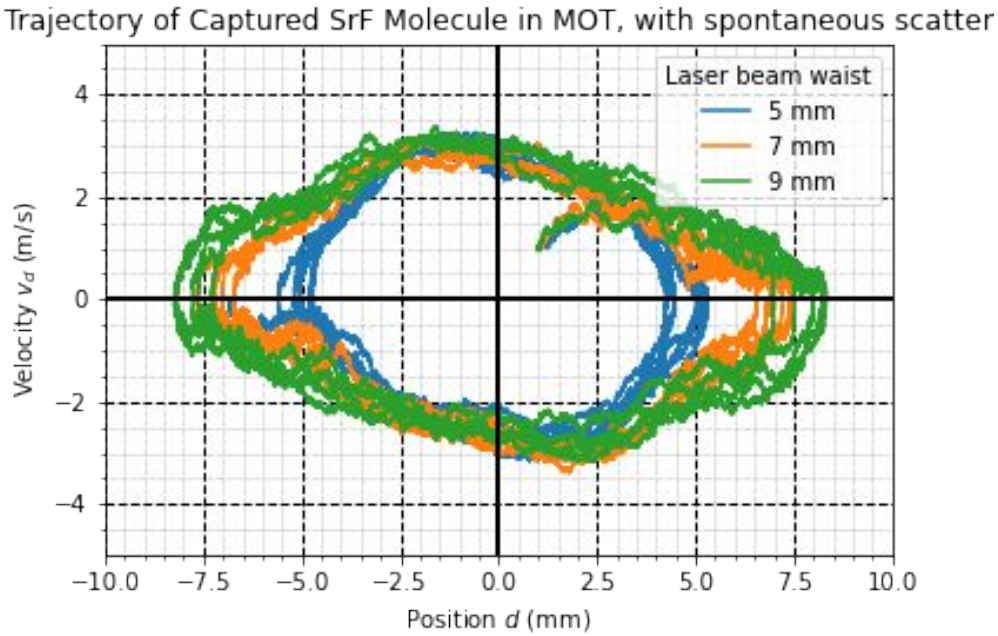




The larger MOT-effective region in d and v_d is evident here for w=9 mm vs. w=5 mm.

SrF MOT performance vs laser beam waist size





Larger capture velocity of MOT as *w* is increased. All MOTs robust to photon scatter in-MOT.

SrF MOT performance vs B-field gradient strength

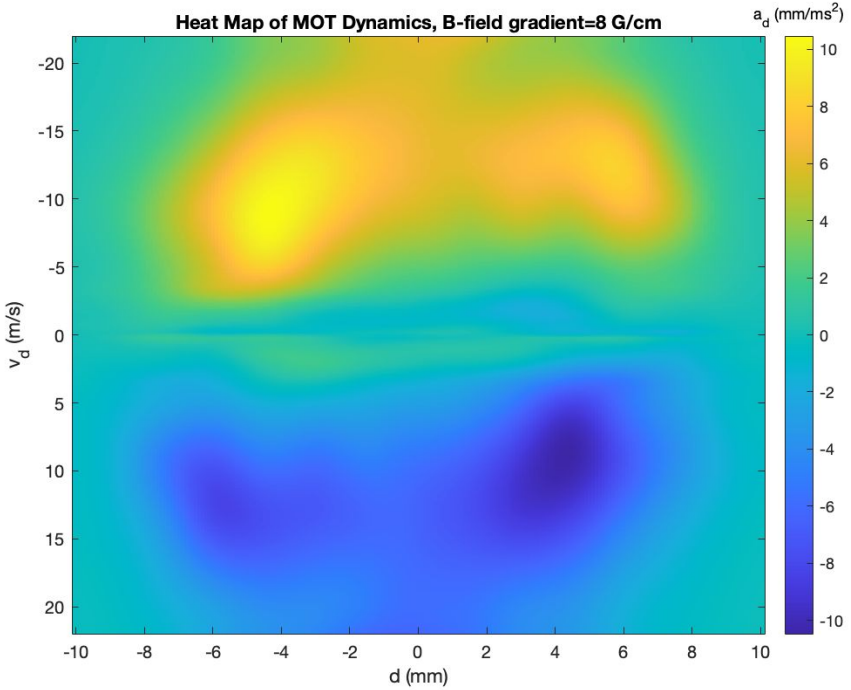
Radial B-field gradient (G/cm)	MOT rms size (mm)	MOT temp (mK)	MOT capture velocity (m/s)
5	5.2	39.0	14.0
8	4.8	36.8	14.1
15	4.1	37.7	12.9

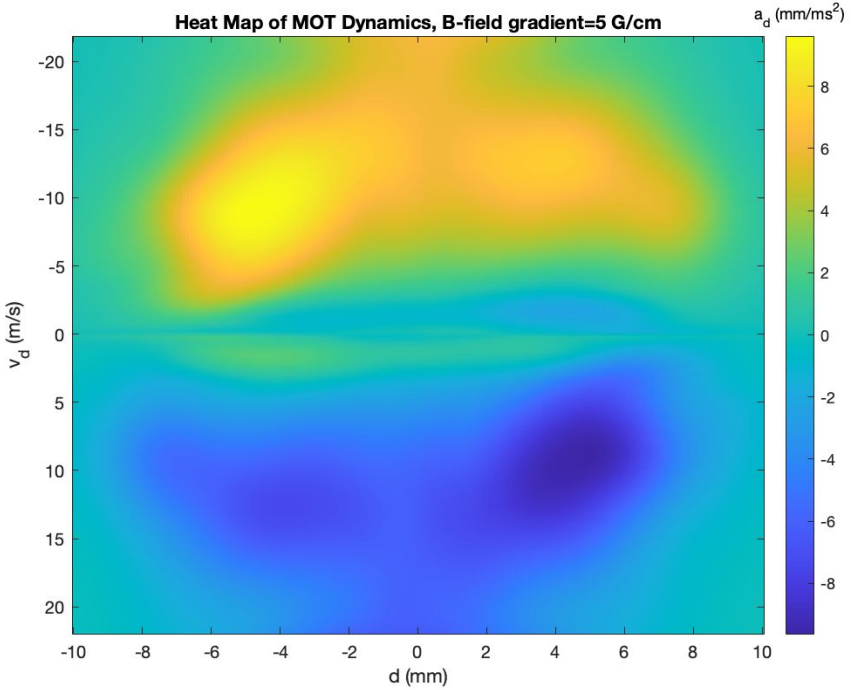
Trend. **As B-field gradient increases:**

- **MOT size decreases** (gradient “compresses” MOT size more)
- **MOT temperature stays roughly the same**
- **MOT capture velocity slightly decreases**

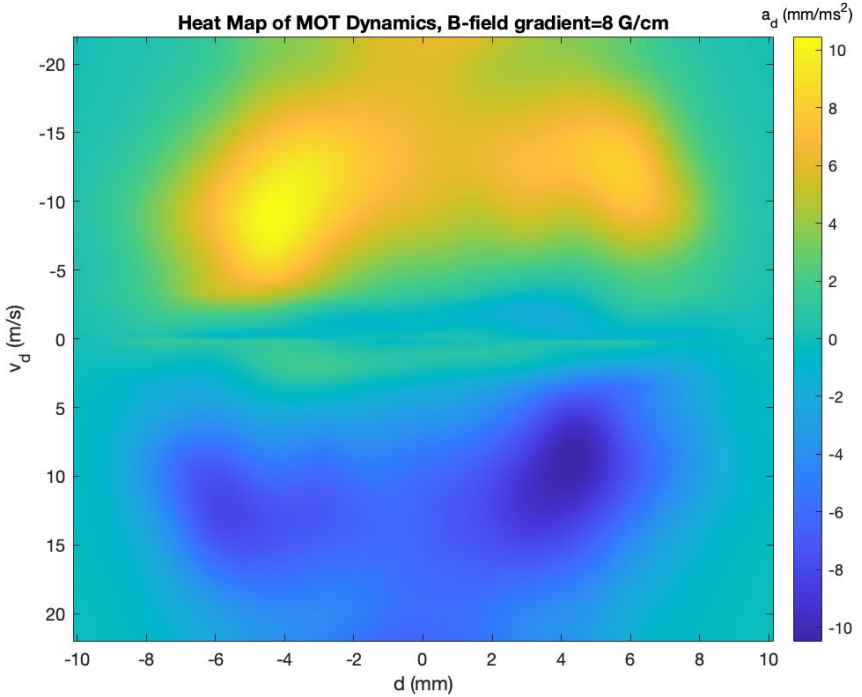
Reasoning: as **MOT B-field gradient is increased**, the **restoring force becomes stronger** at higher displacements from center. This effectively **“compresses” the MOT size** more - which also has the secondary effect of slightly reducing MOT capture velocity.

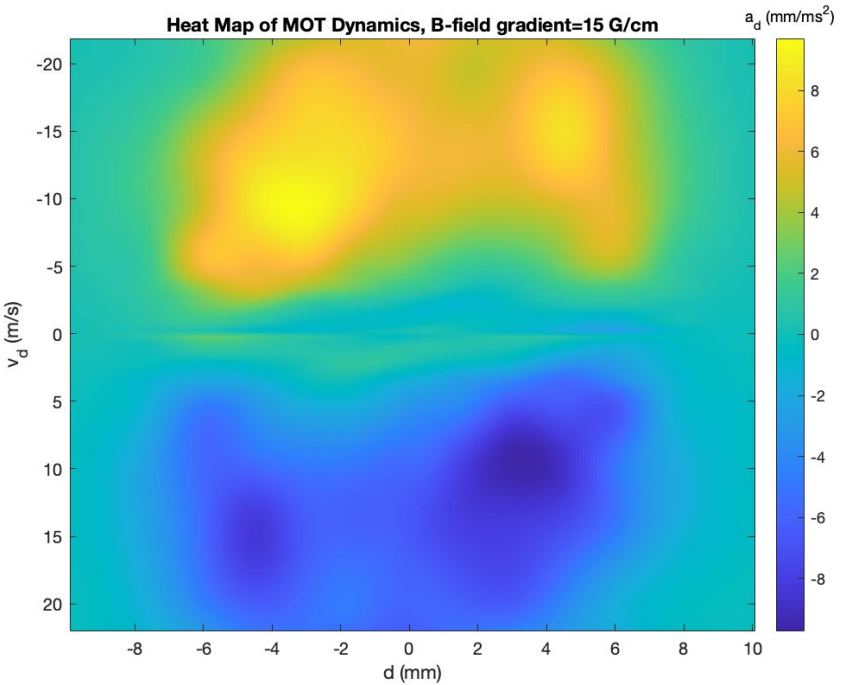
SrF MOT performance vs B-field gradient strength





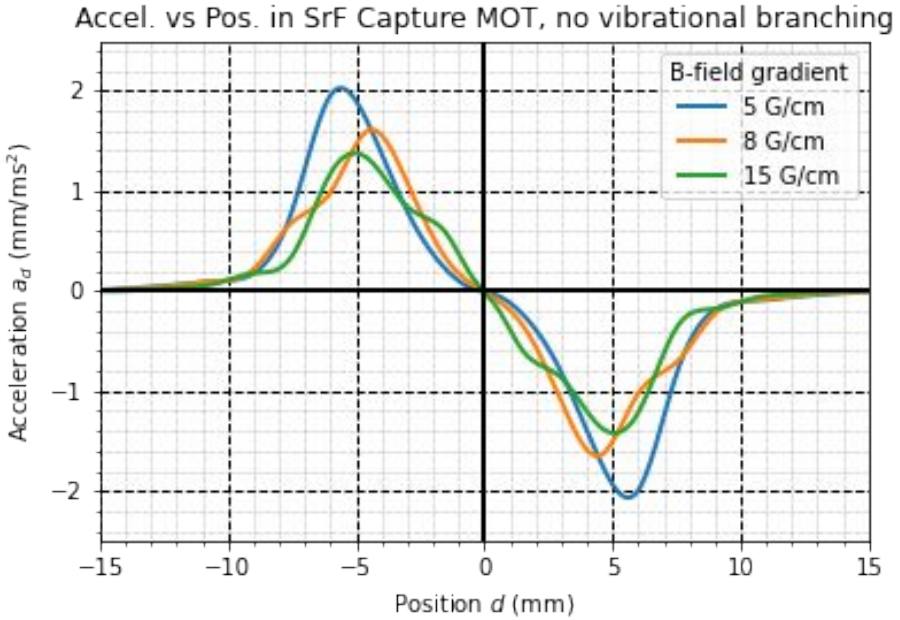
SrF MOT performance vs B-field gradient strength

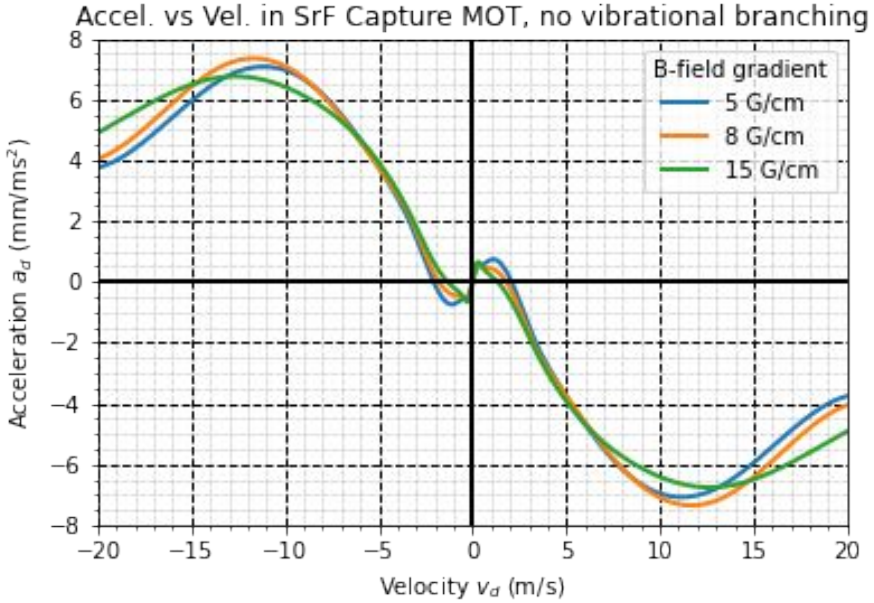




Heat map shows “smaller” effective (d, v_d) region for B-grad=15 G/cm vs. B-grad= 5 G/cm.

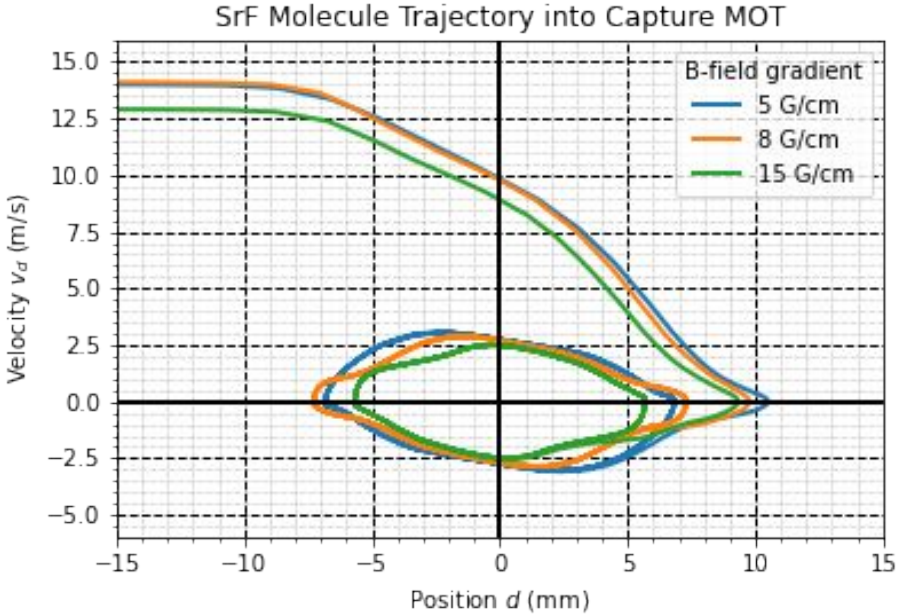
SrF MOT performance vs B-field gradient strength

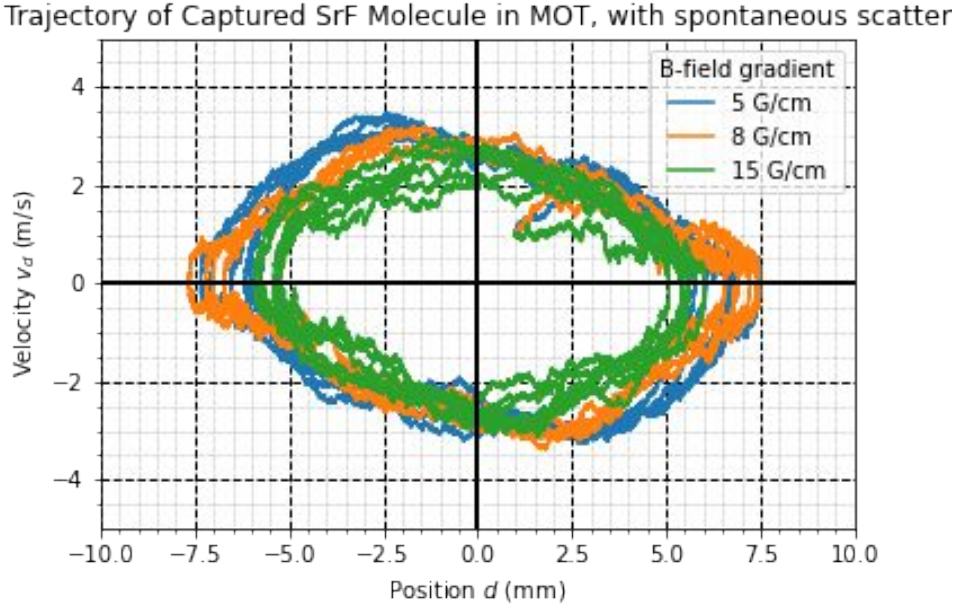




The stronger restoring force at small *d* is evident here for B-grad=15 G/cm vs B-grad=5 G/cm.

SrF MOT performance vs B-field gradient strength





Smaller MOT size for higher B-field gradient. All MOTs robust to photon scatter in-MOT.

SrF MOT performance vs laser beam saturation parameter

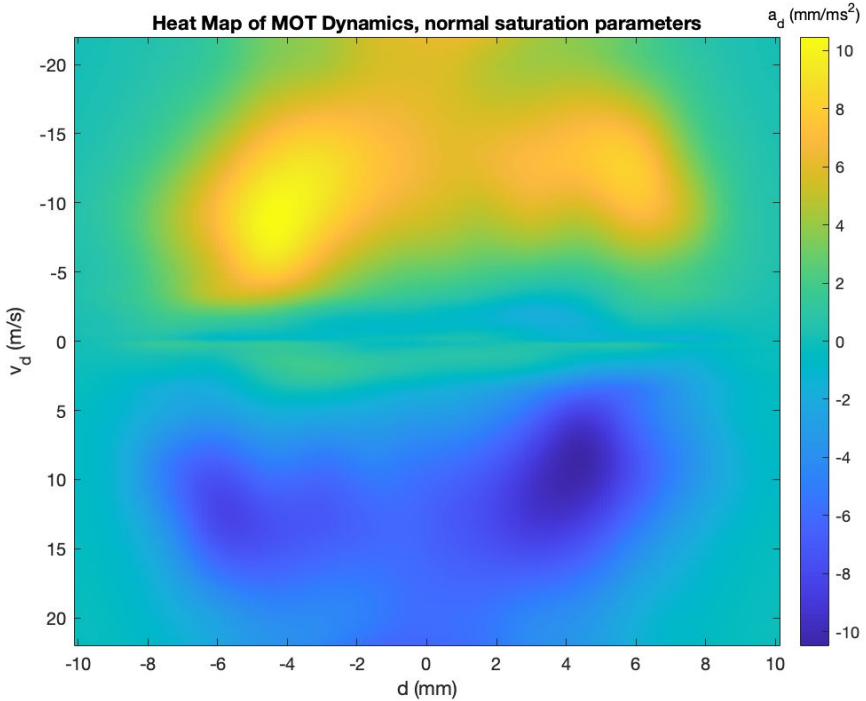
Saturation Parameter [F=1↓,F=0,F=1↑b,F=2, F=1↑r]	MOT rms size (mm)	MOT temp (mK)	MOT capture velocity (m/s)
[10, 20, 10, 31.3, 8.7]	4.8	36.8	14.1
[5, 10, 5, 15.65, 4.35]	4.4	39.4	12.9
[1, 2, 1, 3.13, 0.87]	3.6	18.0	7.5

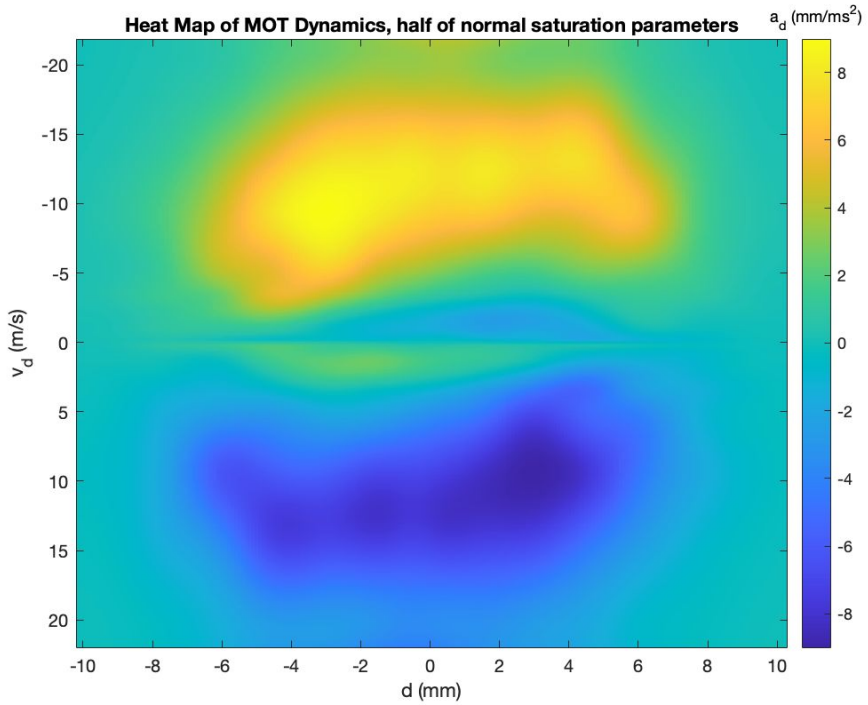
Trend. **As saturation parameter is decreased:**

- **MOT size decreases**
- **MOT temperature decreases**
- **MOT capture velocity decreases a lot**

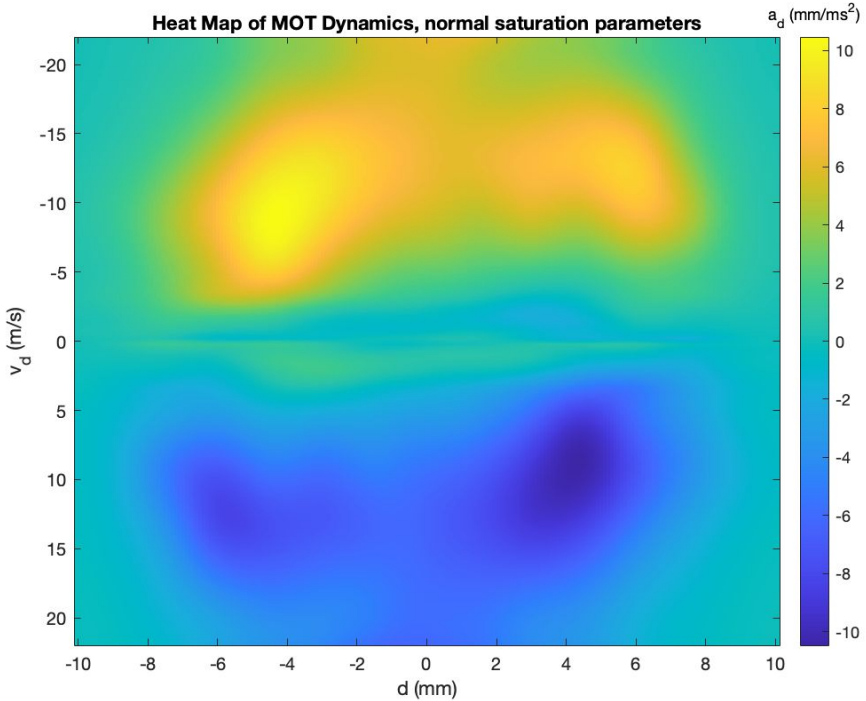
Reasoning: as **saturation parameter is decreased**, less laser power is delivered to MOT. This reduces MOT forces (hence lower capture velocity), but also leads to less heating from photon scatter (hence lower size and temperature).

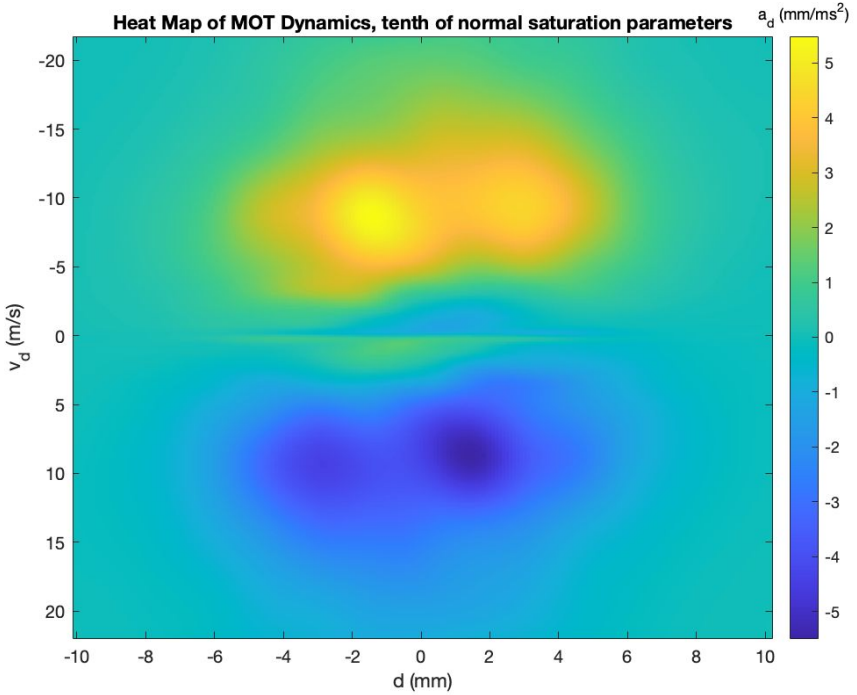
SrF MOT performance vs laser beam saturation parameter





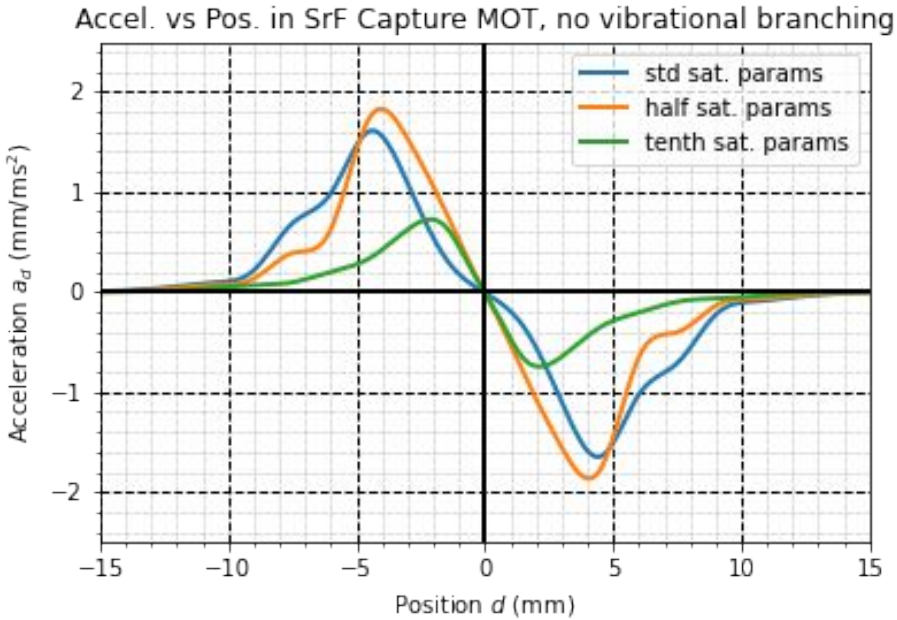
SrF MOT performance vs laser beam saturation parameter

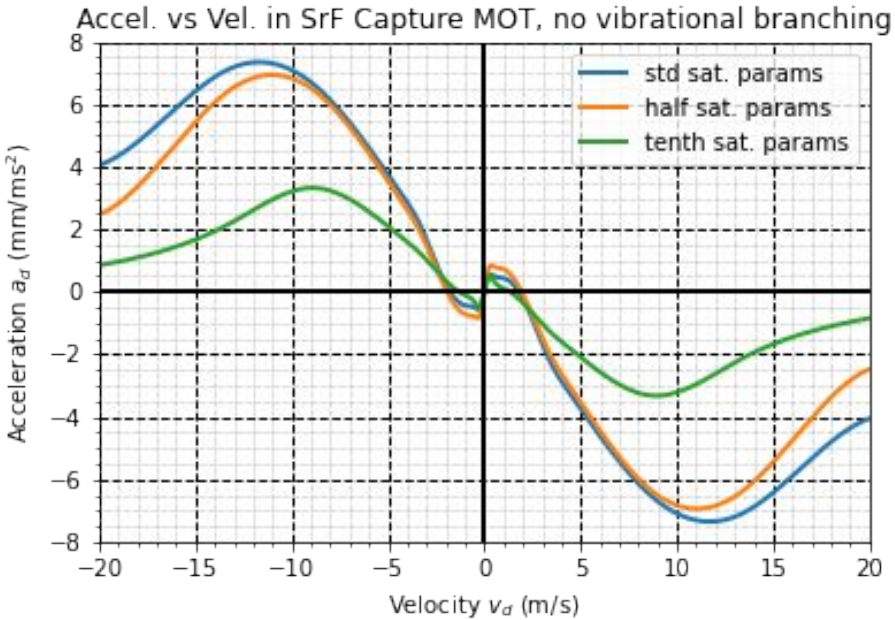




Heat map shows “smaller” effective (d, v_d) region for normal sat. param vs. 1/10 normal.

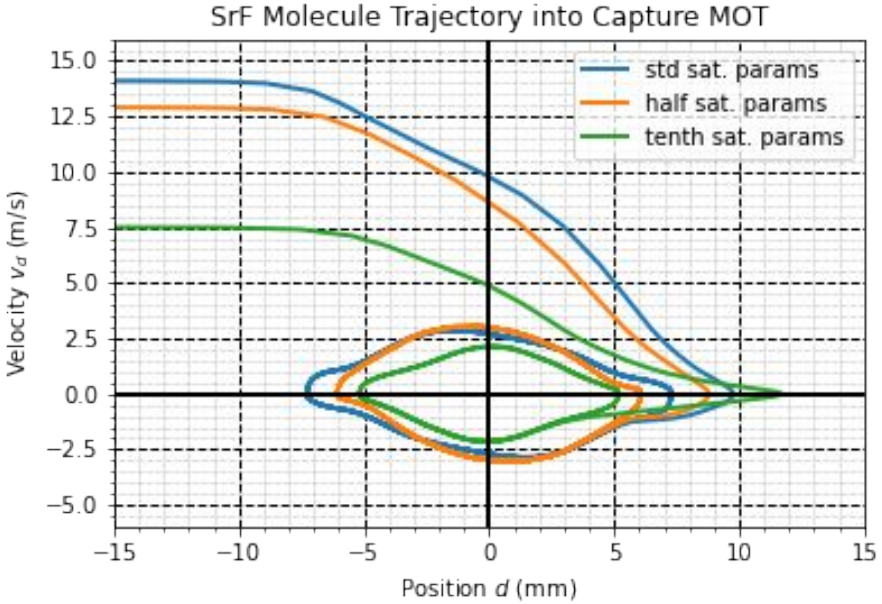
SrF MOT performance vs laser beam saturation parameter

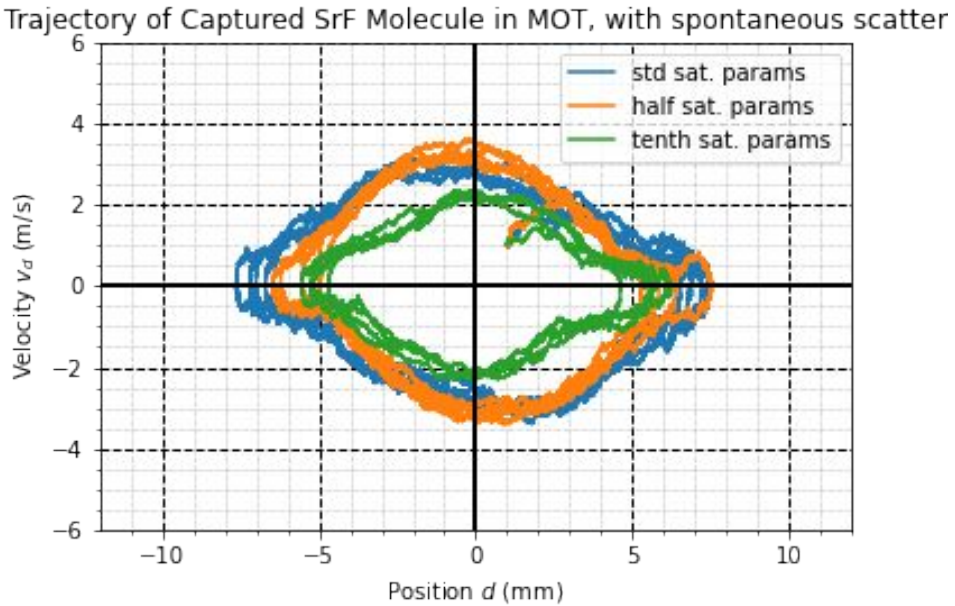




Weaker MOT forces in (d, v_d) evident for 1/10 std. sat. params vs. std. sat. params.

SrF MOT performance vs laser beam saturation parameter





Much weaker capture velocity of MOT as sat. params are decreased.
All MOTs robust to photon scatter in-MOT.

Is the dual-frequency mechanism necessary?

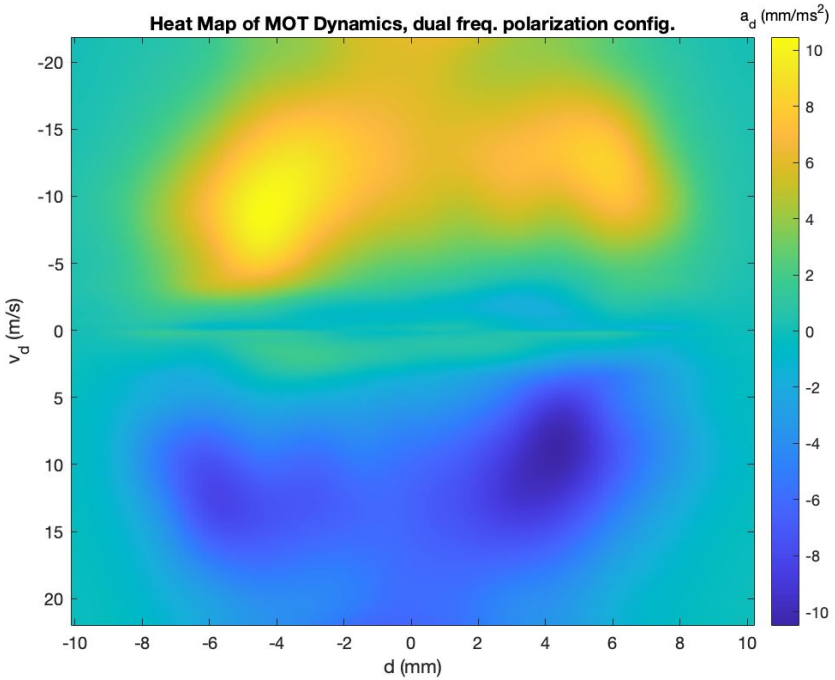
Polarizations [F=1↓,F=0,F=1↑b,F=2, F=1↑r]	MOT rms size (mm)	MOT temp (mK)	MOT capture velocity (m/s)
[+1, +1, +1, -1, -1]	4.8	36.8	14.1
[+1, +1, +1, +1, +1]	5.3	22	10.4

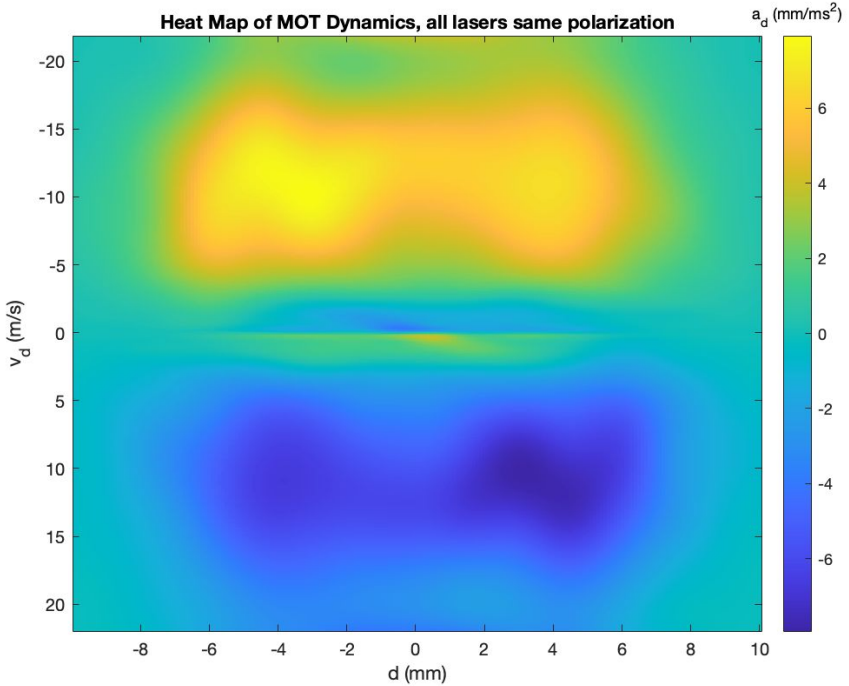
Trend. **If dual-freq mech. is replaced w/all beams have same polarizations:**

- **Weak MOT still exists, albeit not a robust one**
- **Larger MOT size, lower MOT temperature, lower MOT capture velocity**

Reasoning: **If dual frequency mechanism is eliminated**, many **more dark ground states exist in optical cycling** scheme. This leads to **reduced MOT forces** and a **much less robust MOT**. Because of reduced forces, we end up with **larger MOT size**, **lower MOT temperature** due to **less photon scattering**, and **lower capture velocity.**

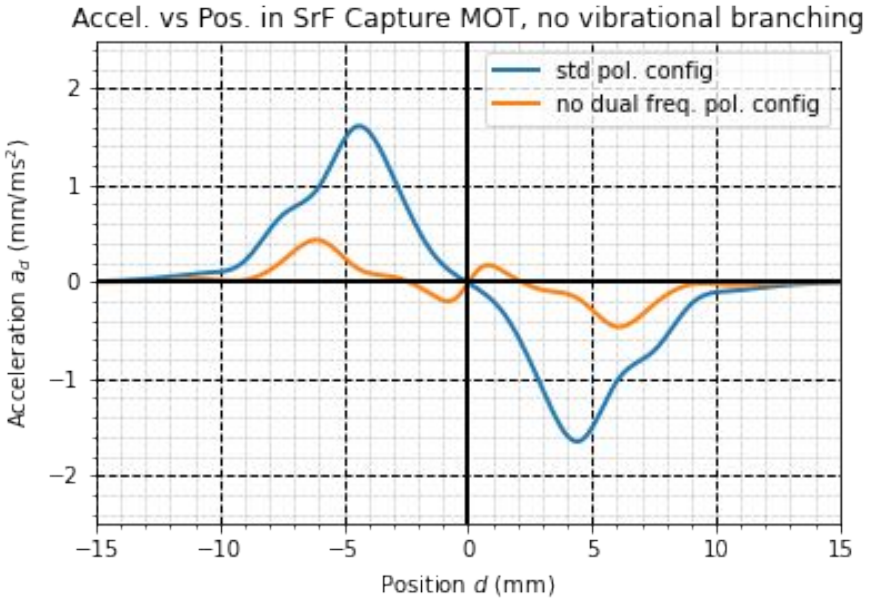
Is the dual-frequency mechanism necessary?

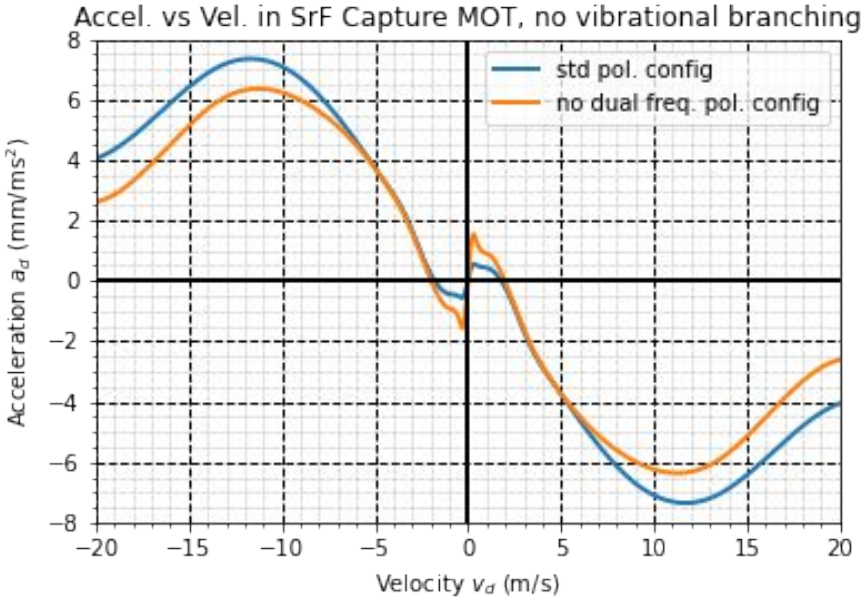




Heat map shows much smaller a_d for entire (d, v_d) range for no dual freq vs. having dual freq.

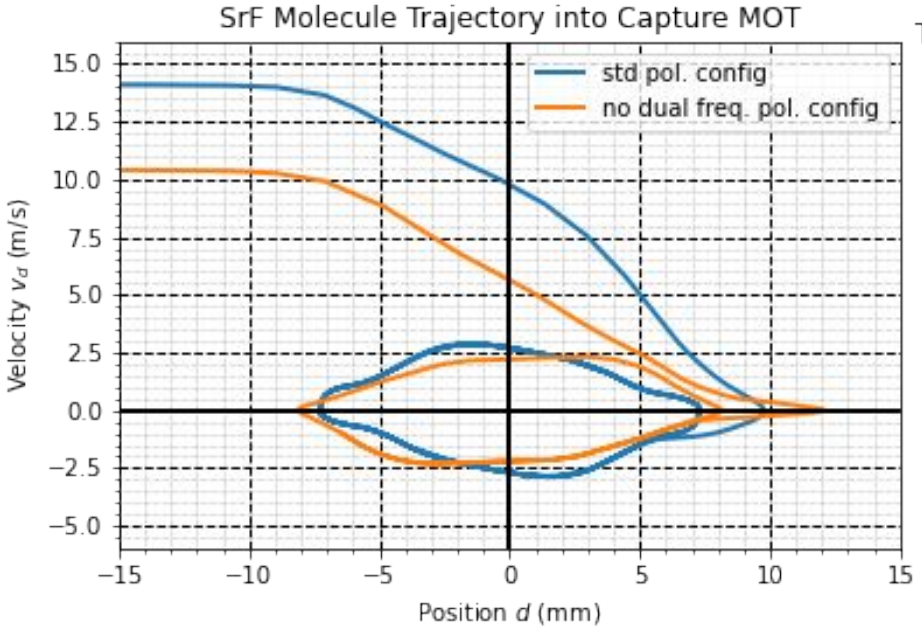
Is the dual-frequency mechanism necessary?

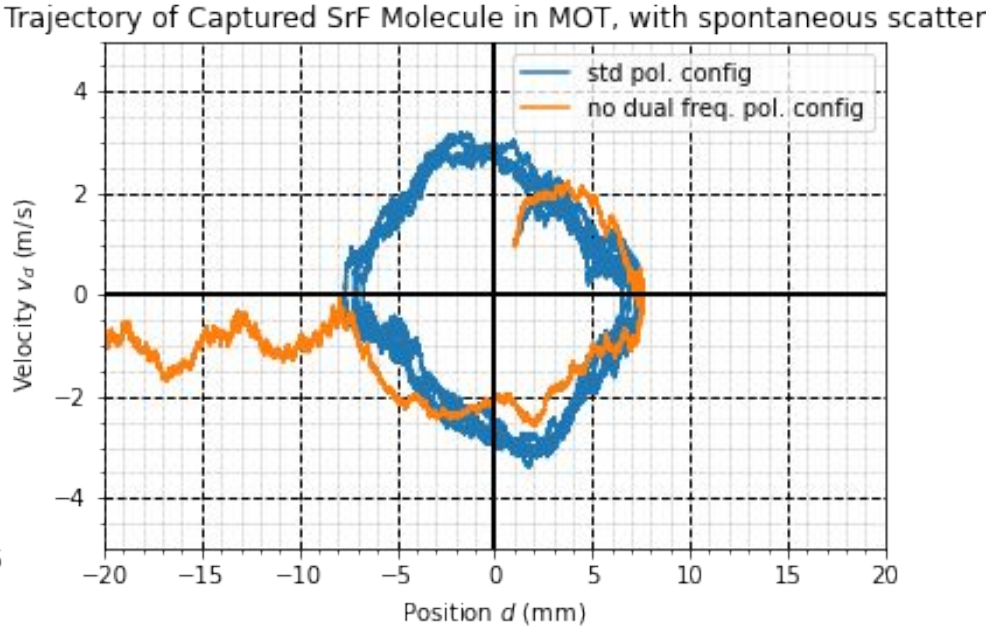




MOT forces much weaker for no-dual-freq mech vs dual-freq mech. There is also stronger sub-Doppler heating and even anti-trapping at small *d* when no dual-freq mech is used.

Is the dual-frequency mechanism necessary?





Capture velocity of MOT is weaker when no dual freq polarization mechanism is used.
Furthermore, the MOT does not even seem to be robust to photon scatter in that case.

Is capture MOT destroyed for all-blue detuning?

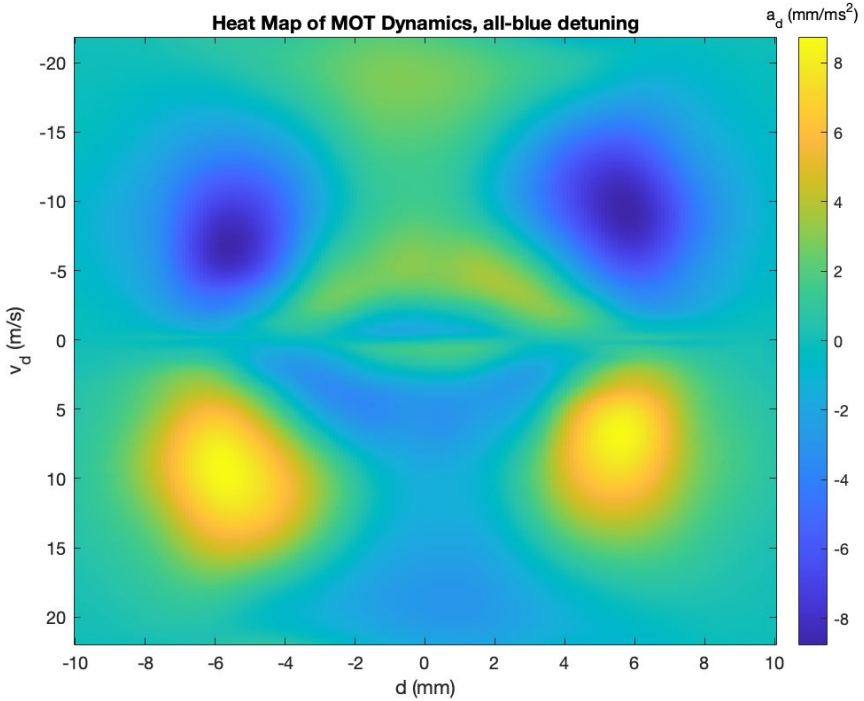
Laser Freqs [F=1↓,F=0,F=1↑b,F=2, F=1↑r]	MOT rms size (mm)	MOT temp (mK)	MOT capture velocity (m/s)
[-1.1Γ, -9.7Γ, -18.5Γ, -26.6Γ, -20.7Γ]	4.8	36.8	14.1
[+1.1Γ, -5.2Γ, -18.6Γ, -25.0Γ, -18.4Γ]	N/A	N/A	N/A

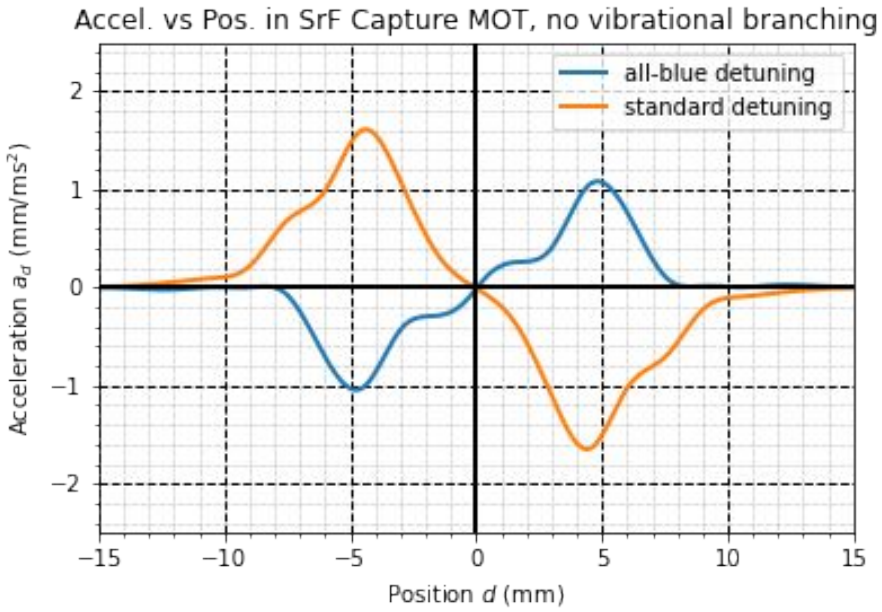
Trend. **If use all-blue detuned lasers for MOT:**

- **All-blue frequencies obtained by "reflecting" their detuning across their relevant hyperfine level** (except for F=1↑b, which is already blue-detuned).
- **All-blue detuning leads completely to anti-trapping and heating behavior of MOT.**

Reasoning: **All-blue detuning reverses sign of trapping and cooling forces in MOT, which leads to anti-trapping and heating, as expected.**

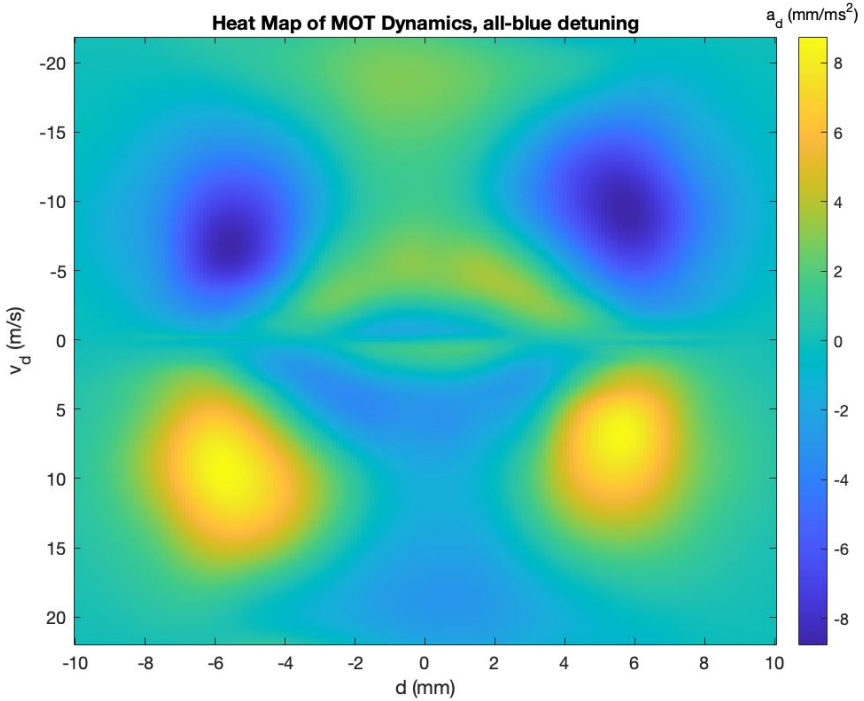
Is capture MOT destroyed for all-blue detuning?

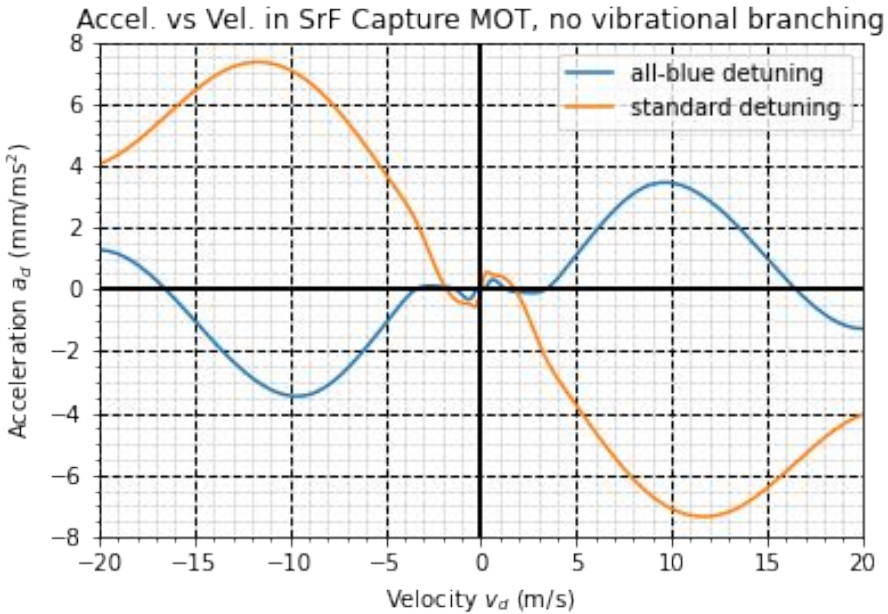




Yes. We observe completely inverted dynamics for cooling and trapping.

Is capture MOT destroyed for all-blue detuning?





No trapping of molecules possible. Capture velocity = 0 m/s.

SrF MOT vs CaF MOT with NO vibrational branching

Molecule (no vibrational repumping)	MOT rms size (mm)	MOT temp (mK)	MOT capture velocity (m/s)
SrF	4.8	36.8	14.1
CaF	6.6	78.4	18.1

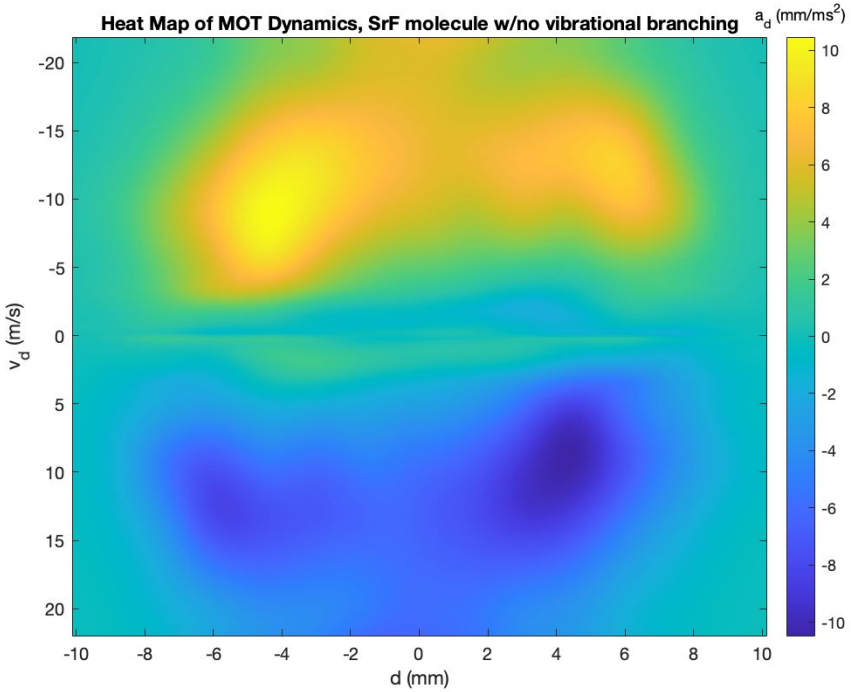
Here, **my canonical settings** (not from TKL *NJP* paper) are **used for both molecules**.

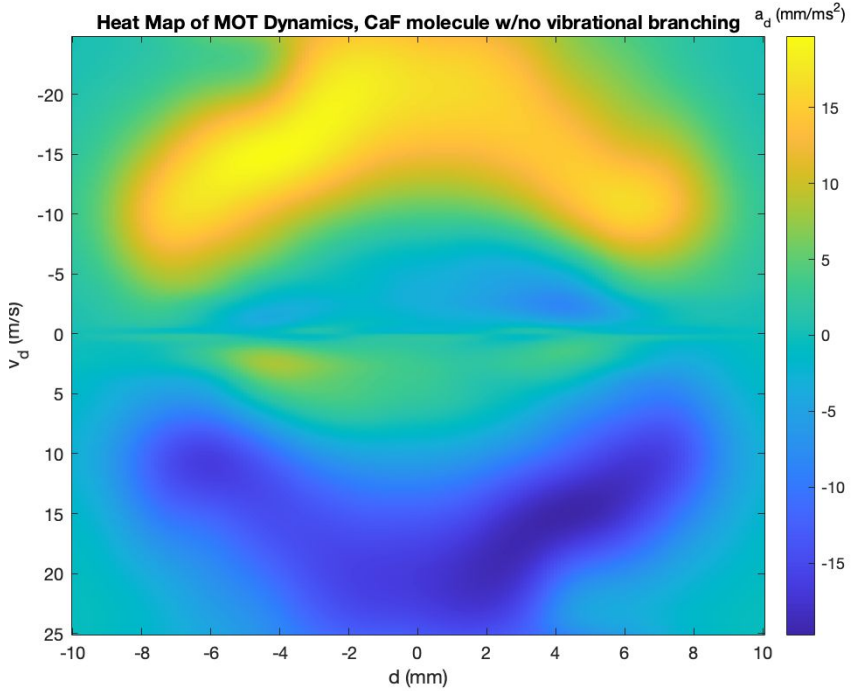
Trend:

- **SrF MOT smaller, lower temperature, lower capture velocity compared to CaF MOT.**

Reasoning: **SrF is heavier than CaF** and has **longer wavelength for principal optical cycling transition**. Therefore, **SrF MOT scattering forces should be weaker**, leading to larger size, lower temp., and lower capture velocity. Further, we **expect numbers above to be further reduced in presence of vibrational branching to v=1.**

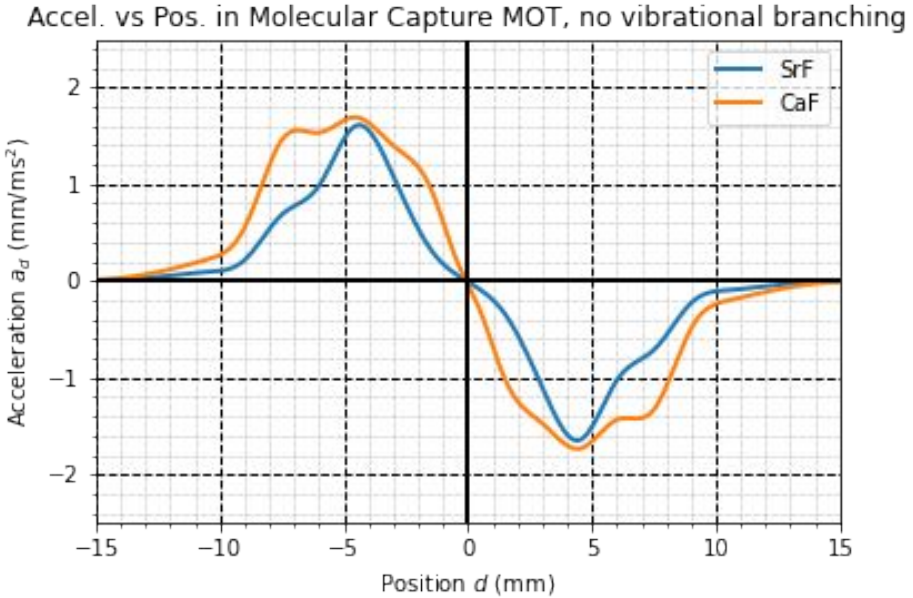
SrF MOT vs CaF MOT with NO vibrational branching

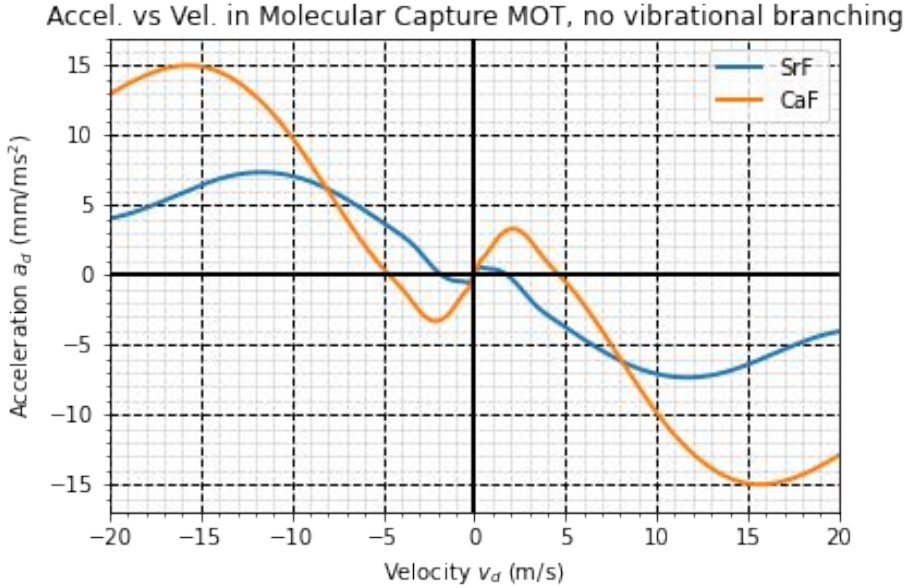




Heat map shows much larger a_d for entire (d, v_d) range for CaF compared to SrF molecules.

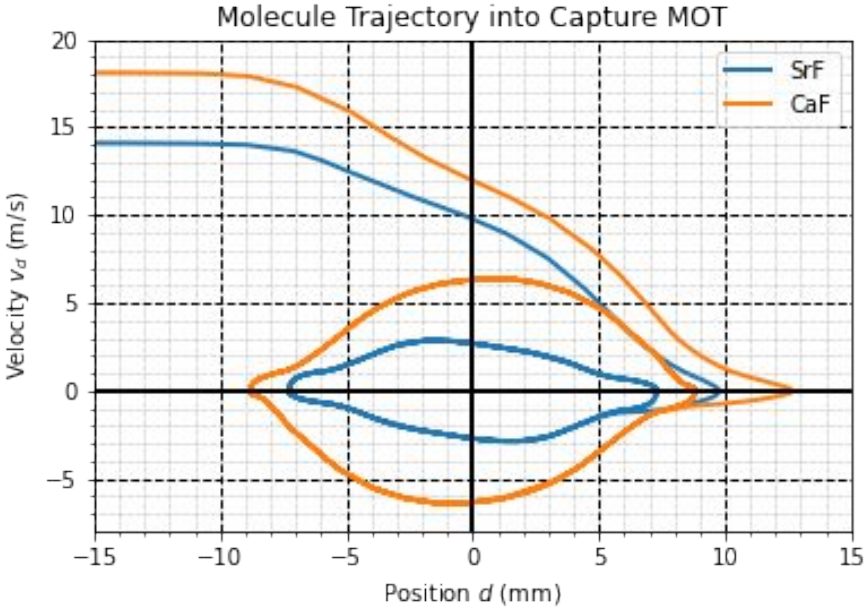
SrF MOT vs CaF MOT with NO vibrational branching

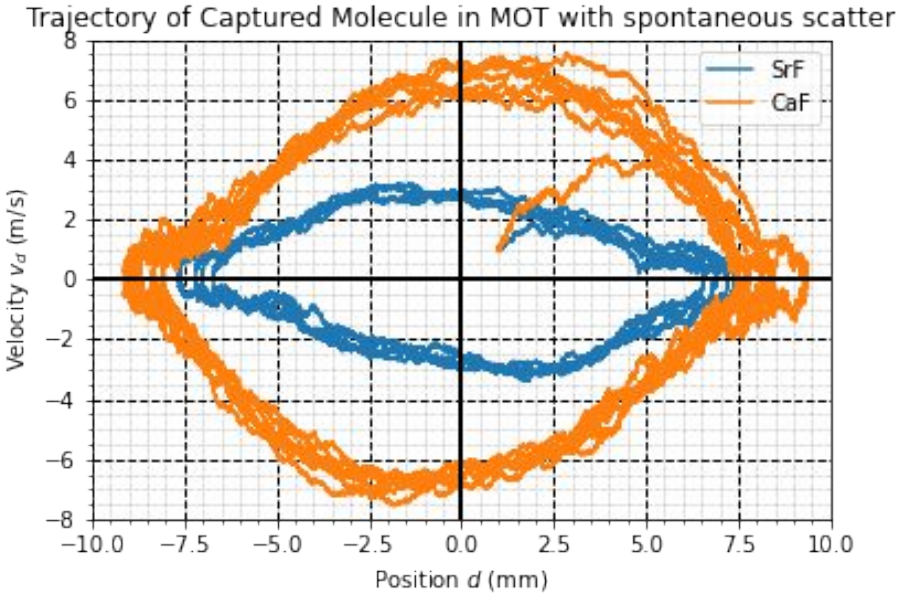




MOT forces much stronger for CaF vs SrF, especially in the v_d domain. Consequently, there is much larger sub-Doppler heating for CaF compared to SrF at low velocities.

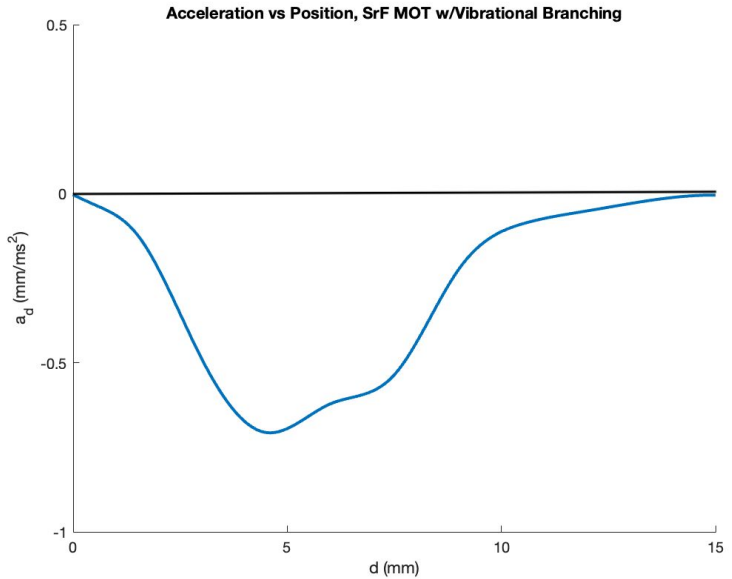
SrF MOT vs CaF MOT with NO vibrational branching





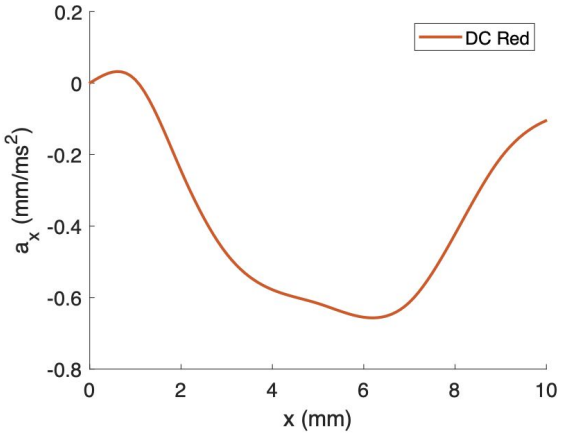
Capture velocity of MOT is much stronger for CaF compared to SrF. Both SrF and CaF MOT are robust to photon scatter, but CaF MOT is much larger in size due to sub-Doppler heating.

SrF MOT w/vib. branching (cf. TKL paper, VRJ Thesis)

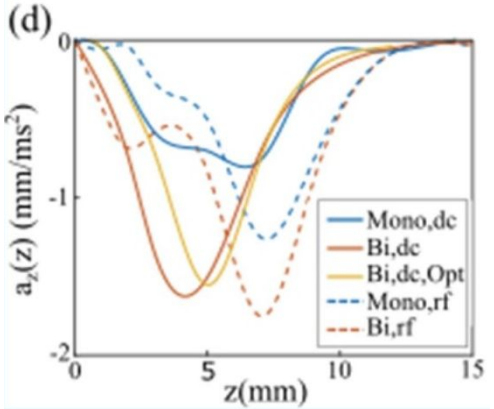


a_d vs. d curve from my simulation run

All results match pretty well!



From VRJ thesis

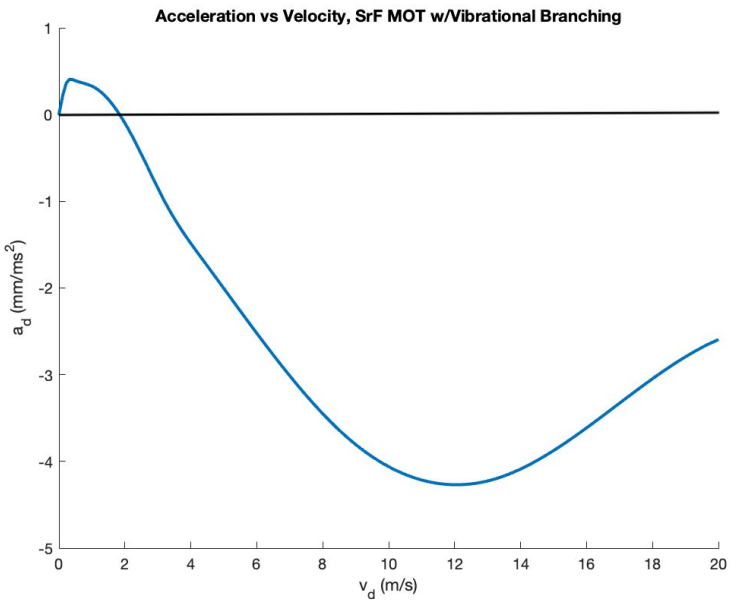


From TKL paper

Label	Transition	s_j	$\Delta_{F,F'}(\Gamma)$	$\hat{p}$
Mono dc	$X \rightarrow A$ (all)	10	$\Delta_{1\downarrow,1'} = -1.1$	σ^-
		20	$\Delta_{0,1'} = -2.3$	σ^-
		8.7	$\boldsymbol{\Delta_{1\uparrow,1'} = -1.2}$	$\boldsymbol{\sigma^+}$
		31.3	$\Delta_{2,1'} = -0.9$	σ^+
		10	$\boldsymbol{\Delta_{1\uparrow,1'} = +1}$	$\boldsymbol{\sigma^-}$

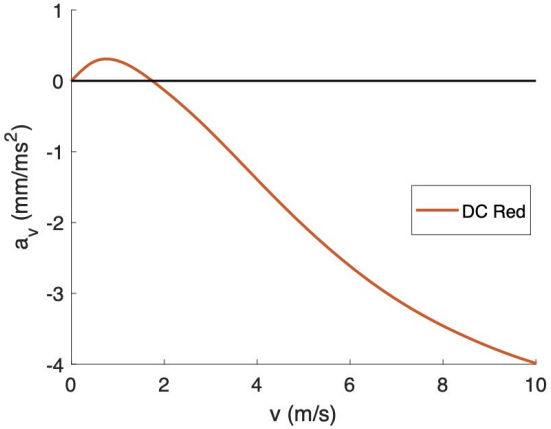
Parameters for simulation (from TKL paper)

SrF MOT w/vib. branching (cf. TKL paper, VRJ Thesis)

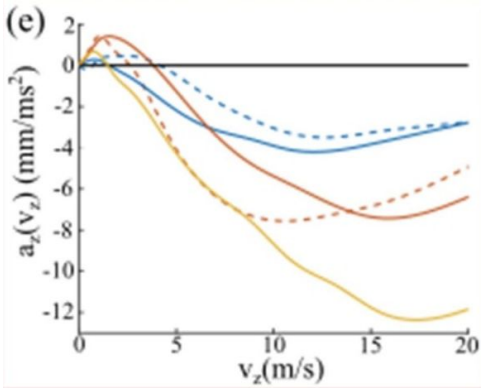


a_d vs. v_d curve from my simulation run

All results match pretty well!

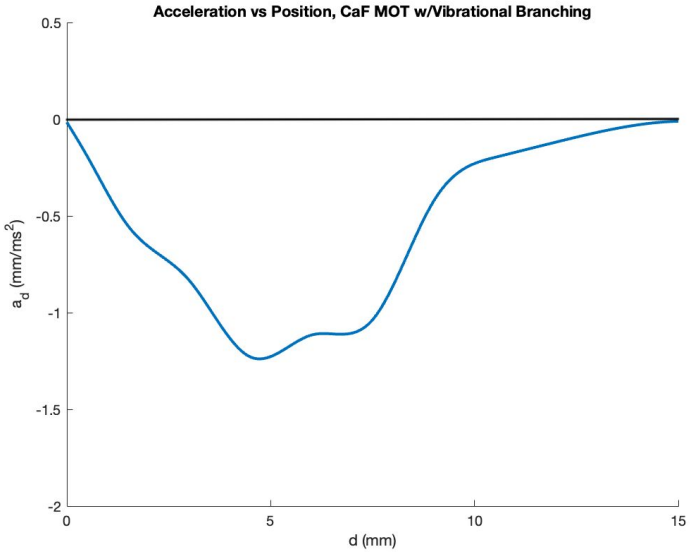


From VRJ thesis

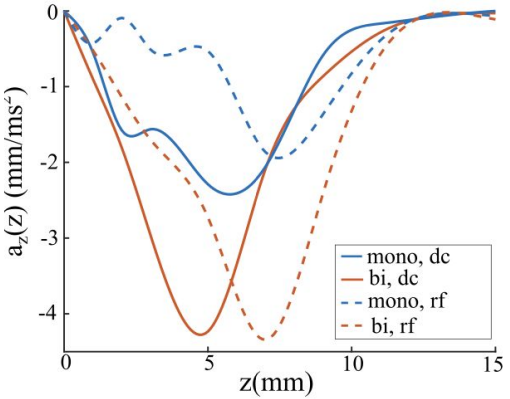


From TKL paper (blue indicates X-A MOT)

CaF MOT with vibrational branching (cf. TKL paper)



a_d vs. d curve from my simulation run



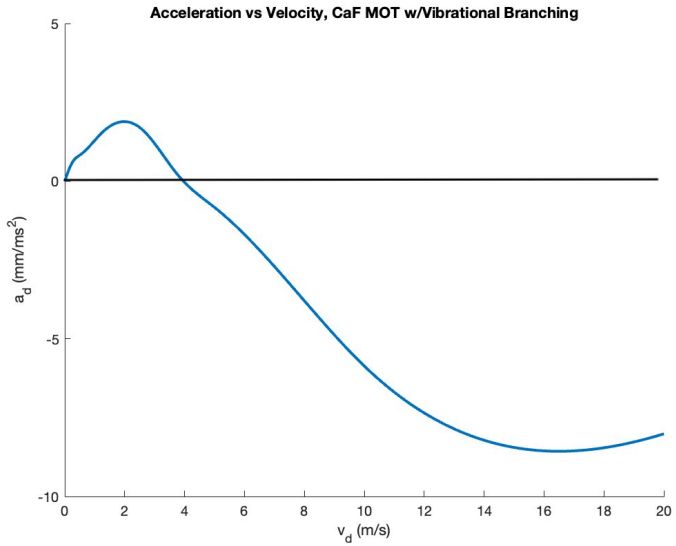
From TKL paper. Parameters for simulation from TKL paper (below)

CaF MOT configurations simulated with OBEs

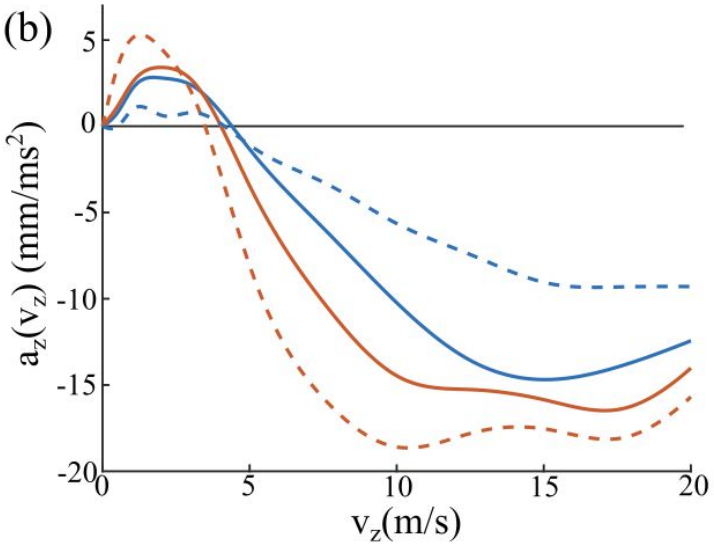
Label	Transition	$s_{j,Max}$	$\Delta_{F,F'}(\Gamma)$	$\hat{p}$
Mono,dc	$X \rightarrow A$ (all)	20	$\Delta_{1\downarrow,1'} = -1.4$	σ^-
		20	$\Delta_{0,1'} = -1.4$	σ^-
		20	$\boldsymbol{\Delta_{1\uparrow,1'} = -1, \Delta_{2,1'} = +2}$	$\boldsymbol{\sigma^-}$
		20	$\boldsymbol{\Delta_{2,1'} = -1.4}$	$\boldsymbol{\sigma^+}$

TKL results for a_d vs d show stronger deceleration for CaF compared to mine.
But, in both cases, MOT forces in CaF are stronger compared to SrF.

CaF MOT with vibrational branching (cf. TKL paper)



a_d vs. v_d curve from my simulation run



From TKL paper (blue indicates X-A MOT)

TKL results for a_d vs v_d also show stronger deceleration for CaF compared to mine.
But, in both cases, MOT forces in CaF are stronger compared to SrF.

SrF MOT vs CaF MOT WITH vibrational branching

Molecule (with vibrational repump)	MOT rms size (mm)	MOT temp (mK)	MOT capture velocity (m/s)
SrF	5.0	31.1	9.3
CaF	7.4	54.6	12.6

Here, **TKL *NJP* (2023) paper settings** are **used for both molecules.**

Trend:

- **Even for vibrational branching to v=1, SrF MOT is weaker than CaF MOT (SrF MOT is smaller, has lower temperature, and lower capture velocity).**
- Calculated values above match closely with results in TKL *NJP* (2023) paper (see next slide).

Reasoning: Even if we **include vibrational branching to v=1** and have vibrational repumper, **extra dark states impact SrF and CaF equally**. So, **all things being equal, CaF has stronger MOT forces** compared to SrF because of **lighter weight and stronger scattering force on principal optical cycling transition**.

SrF MOT vs CaF MOT WITH vibrational branching

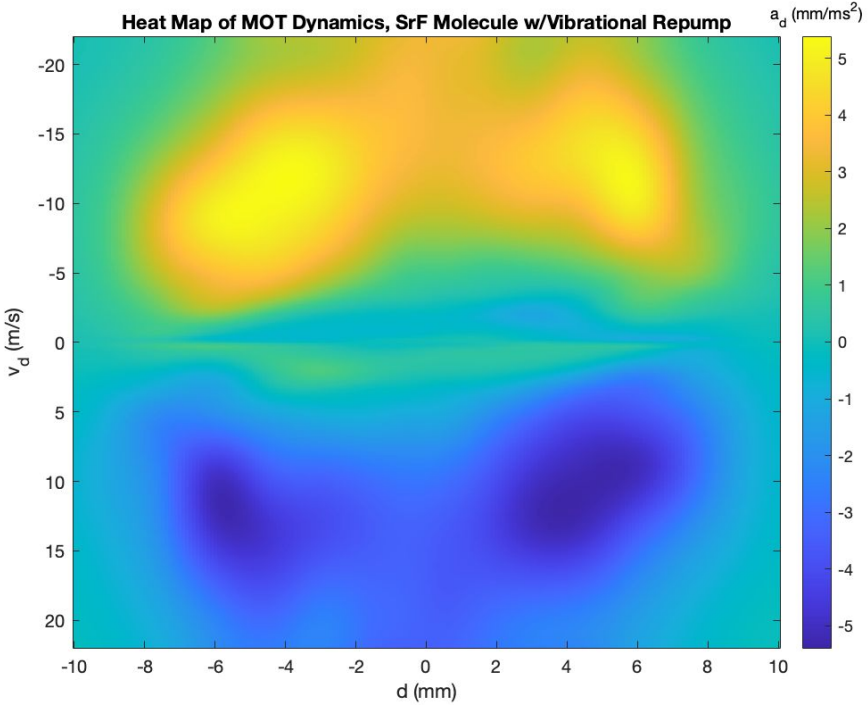
Here are the results from TKL *NJP* (2023) paper for SrF and CaF X-A MOTs:

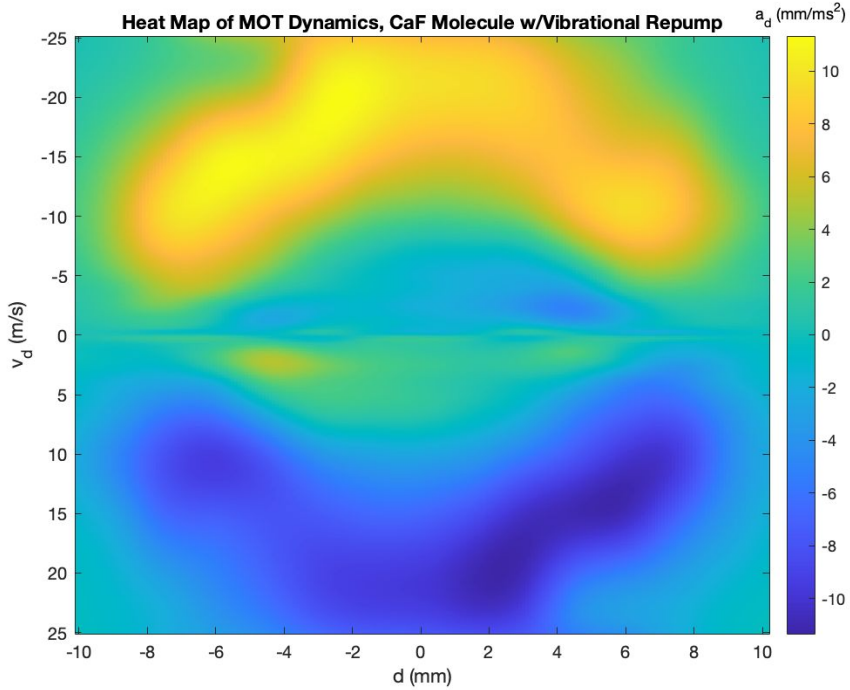
SrF redMOT configurations			
Label	v_{cap}	T (mK)	σ (mm)
Mono,dc	8.6	23	4.8

CaF redMOT configurations			
Label	v_{cap}	T (mK)	σ (mm)
Mono,dc	12.2	50	7.4

Values for v_{cap}, T, and σ all match between my simulation run and TKL's results, for SrF and CaF MOTs.

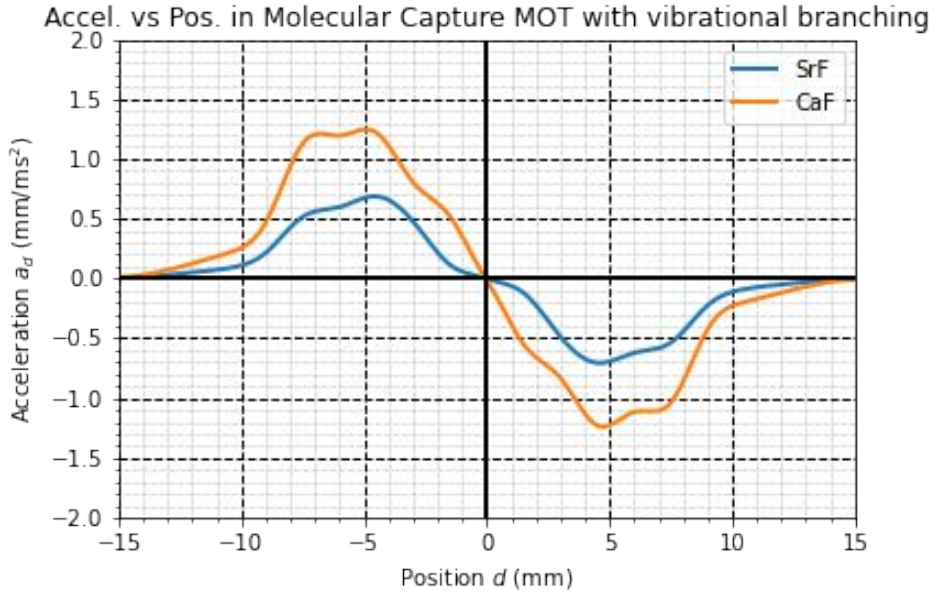
SrF MOT vs CaF MOT WITH vibrational branching

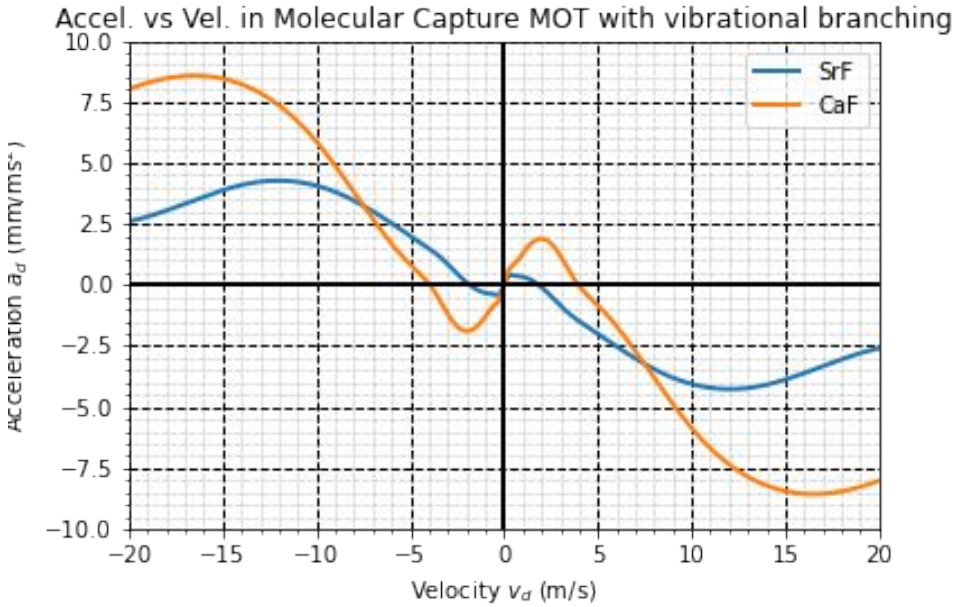




Heat map shows much larger a_d for entire (d, v_d) range for CaF compared to SrF molecules, even in presence of vibrational branching and repumping.

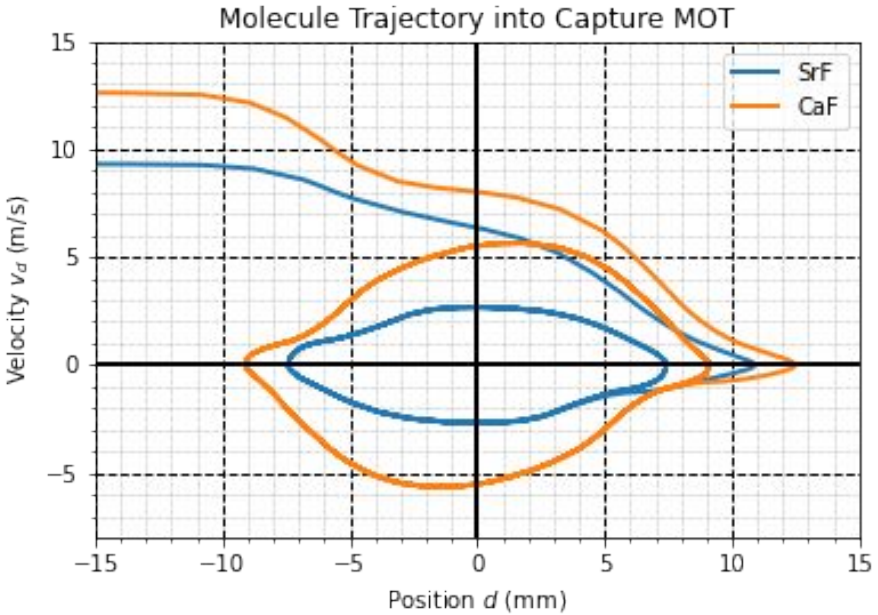
SrF MOT vs CaF MOT WITH vibrational branching

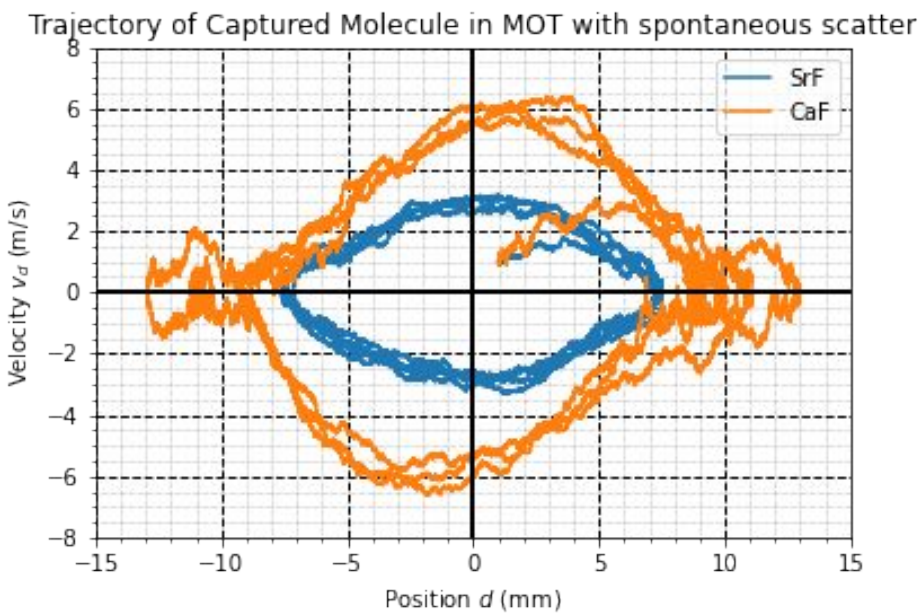




MOT forces still much stronger for CaF vs SrF, for both d and v_d domains, even when incorporating vibrational branching. There is still much larger sub-Doppler heating for CaF compared to SrF at low velocities.

SrF MOT vs CaF MOT WITH vibrational branching





Capture velocity of MOT is still much stronger for CaF compared to SrF, even when incorporating vibrational branching. SrF MOT is still robust to photon scatter, CaF seems mostly robust, but strong sub-Doppler heating could lead to instability.

Grand Summary of Molecular MOT Results

- **My SrF capture red-MOT results**, when **including vibrational branching to v=1**, **match TKL paper** and VRJ thesis results closely (**T ≈ 30 mK, σ ≈ 5 mm, v_{cap} ≈ 9 m/s**).
- Trials of molecular MOT behavior reveal results commensurate with what we expect from theory of MOTs:
  - **Larger MOT beam** leads to **better molecule capture** at **cost of larger, hotter MOT.**
  - **Larger B-field gradient decreases equilibrium size** of MOT.
  - **Lower saturation parameter** drastically **reduces temperature**, at **cost of weaker capture forces and smaller MOT**.
- **Trials above validate the procedure of compressed MOT** after capture - **increase B-field gradient and lower MOT beam intensity to make MOT smaller and colder.**
- **Sanity checks of molecular MOT** behavior reveal **simulations capture expected physics**:
  - **Dual-frequency polarization mechanism is needed** for robust molecular MOTs.
  - **Red-detuning of laser frequencies is needed** for MOT to work in first place.
- **SrF MOT is weaker than CaF MOT** (w/ and w/o vibrational branching) b/c **SrF is heavier and optical cycling wavelength is longer** - this leads to weaker MOT trapping and cooling forces.
- **All normal molecular MOTs** simulated are **robust to photon scatter in-MOT**
- Most importantly - the **molecular MOT OBE simulation code is "molecule agnostic"**, so it's **easy to swap out molecule parameters to compare results** across molecular species.

References

1. T K Langin and D DeMille, “Towards Improved Loading, Cooling, and Trapping of Molecules in Magneto-Optical Traps”, *New J. Phys.* **25** (2023) 043005.
    a. Referred to as TKL *NJP* (2023) paper in slides.
2. V R Jorapur, “Towards a Bose-Einstein Condensate of SrF Molecules”, PhD thesis, Yale University (2024).
    a. Referred to as VRJ thesis (2024) in slides.