Characterizing the Optical Trapping of Rare Isotopes by Monte Carlo Simulation

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Optical trapping techniques are an efficient way to probe limited quantities of rare isotopes. In order to achieve the highest possible measurement precision, it is critical to optimize the optical trapping efficiency. This work presents the development of a three-dimensional semi-classical Monte Carlo simulation of the optical trapping process and its application to optimizing the optical trapping efficiency of Radium for use in the search of the permanent electric dipole moment of $^{225}$Ra. The simulation includes an effusive-oven atomic beam source, transverse cooling and Zeeman slowing of an atomic beam, a three-dimensional magneto-optical trap, and additional processes such as collisions with residual gas molecules. We benchmark the simulation against a well-characterized $^{88}$Sr optical trap before applying it to the $^{225}$Ra optical trap. The simulation reproduces the relative gains in optical trapping efficiency measured in both the $^{88}$Sr and $^{225}$Ra optical traps. The measured and simulated values of the overall optical trapping efficiencies for $^{88}$Sr are in agreement; however, they differ by a factor of 30 for $^{225}$Ra. Studies of several potential imperfections in the apparatus or systematic effects, such as atomic beam source misalignment and laser frequency noise, show only limited effects on the simulated trapping efficiency for $^{225}$Ra. We rule out any one systematic effect as the sole cause of the discrepancy between the simulated and measured $^{225}$Ra optical trapping efficiencies; but, we do expect that a combination of systematic effects contribute to this discrepancy. The accurate relative gains predicted by the simulation prove that it is useful for testing planned upgrades to the apparatus.

I. INTRODUCTION

Optical trapping is now a standard technique in a variety of rare isotope applications such as searches for new physics. Examples include ground water dating with $^{81}$Kr and $^{39}$Ar [1, 2], precision measurements of the charge radii of exotic $^{6}$He nuclei [3, 4], a search for new physics by probing $\beta$-decay in unstable $^{4}$He, $^{21}$Na, $^{37}$K [6, 8], and a search for atomic parity violation in Fr isotopes [9]. Our primary application is using optically trapped $^{225}$Ra in the search for a permanent electric dipole moment (EDM) [10] (for a recent review of EDMs see [11]). $^{225}$Ra offers enhanced sensitivity in diamagnetic atomic EDM searches due to the octupole deformation of its nucleus [12, 13]. Using optically trapped $^{225}$Ra atoms, we have measured the $^{225}$Ra EDM to be $d(225$Ra) < $1.4 \times 10^{-23}$ e·cm [14]. In order to efficiently utilize limited quantities of $^{225}$Ra (10$^{14}$ atoms per measurement) and to further improve the measurement statistical precision, it is essential to optimize the optical trapping efficiency of our experimental apparatus. Since it is impractical to empirically study the effect of a multitude of parameters in our optical trapping system, we have chosen to model the apparatus using a purpose-built three-dimensional Monte Carlo (MC) simulation.

Existing simulations included some, but not all, of the features necessary to fully model our apparatus. Early simulations (ca. 1990) typically only simulated individual subsystems of an optical trapping apparatus, as the available computational resources of the era limited the complexity that could be reasonably modeled. One such MC simulation modeled atomic beam cooling, but approximations, such as assuming isotropic spontaneous emission in the presence of circularly polarized laser beams, only allowed for upper limits on the atomic beam velocity distribution to be obtained [15]. A Langevin-equation based simulation of atoms in one- and three-dimensional optical molasses predicted temperatures of cooled Na and Cs atoms in agreement with experiments, but also produced exotic results such as non-Gaussian velocity distributions [16]. As computational power increased over the following decades, simulations of the laser cooling and trapping process increased in complexity. A two-dimensional simulation [17] used multiple cooling and trapping subsystems chained together to model experiments, but did not include any additional experimental factors, such as the atomic beam source. A recent simulation [18] of the slowing of a supersonic
atomic beam incorporated a three-dimensional treatment of atoms in a laser-field, but did not include atomic beam collimation nor optical trapping. Fully quantum treatments of light-atom interactions [19, 20] used MC wavefunction techniques, but as with earlier simulations, typically only looked at individual subsystems, such as optical molasses.

In the absence of an existing simulation that could fully model our $^{225}\text{Ra}$ optical trap, we developed a laser cooling and trapping MC simulation that includes both the main subsystems of an optical trapping system and additional experimental details of our apparatus such as the atomic beam source. In addition to applying it to our $^{225}\text{Ra}$ optical trap, we benchmarked our simulation against a well-characterized $^{88}\text{Sr}$ optical trap used in an optical lattice clock at JILA. The simulation replicates certain performance characteristics of both optical traps, such as the relative gain in trapping efficiency from transversely cooling the atomic beam, but does not reproduce the measured overall trapping efficiency by a factor of 30 for the $^{225}\text{Ra}$-optical trap.

In this work we present the decade-long development of our MC simulation and its application to our $^{225}\text{Ra}$ optical trap. In Sec. II we describe the experimental setups of the $^{225}\text{Ra}$ and $^{88}\text{Sr}$ optical traps considered in the simulation. Sec. III details the features of the MC simulation. We present the simulation results in Sec. IV and further systematic studies examining the discrepancy between the measured and simulated results in Sec. V. Sec. VI outlines our planned upgrades to and future use of the simulation. Our treatment of light-atom interactions, atomic beam source angular & velocity distributions, and estimates of the relevant van der Waals $C_6$ coefficients are detailed in Appendices A, B, and C respectively.

II. THE OPTICAL TRAPPING SYSTEMS

A. Ra optical trap

The Ra optical trap was developed and optimized at Argonne National Laboratory for use in a next-generation search for a permanent EDM [21, 22]. The optical trap is fully detailed in Refs. 10, 23, 24 and we present here an overview of the subsystems relevant to our simulation. $^{225}\text{Ra}$ ($\tau_{1/2} = 1600$ yr, nuclear spin = 0) is used for testing and optimizing the trap, while $^{225}\text{Ra}$ ($\tau_{1/2} = 15$ d, nuclear spin = 1/2) is used for the EDM measurements.

The lowest-lying $^1S_0 \leftrightarrow ^1P_1$ transition is typically used for laser cooling of alkaline-earth atoms, e.g. Ca and Yb, but we do not use this transition for Ra due to the high probability for an atom to decay into the metastable $D$ and $P$ states. Instead, we use the weaker $7s^2 \, ^1S_0 \leftrightarrow 7s7p \, ^1P_1$ transition near 714 nm for laser cooling and trapping, see Fig. I (left). This intercombination transition is weakly allowed in divalent atoms due to singlet-triplet mixing [25]. For Ra, the $^1P_1$ lifetime is 422 ns [26], yielding a natural linewidth $\gamma_{\text{Ra}}/2\pi \approx 380$ kHz. While this transition is sufficiently strong for trapping Ra atoms [23], we are only able to slow atoms with initial velocities of up to $63 \, \text{m s}^{-1}$.

A diagram of the laser trapping portion of the apparatus is shown in Fig. 2. We heat a crucible containing metallic Ba and Ra(NO$_3$)$_2$ to about 500 °C, sufficient to produce a beam of atomic Ra (chemically reduced by the Ba) that we collimate with a nozzle of length $L_{\text{noz}} = 8.3 \, \text{cm}$ and diameter $d_{\text{noz}} = 0.2 \, \text{cm}$. At this temperature, we determine the total integrated beam flux to be $5 \times 10^9 \, \text{s}^{-1}$ by collecting laser-induced fluorescence on a photomultiplier tube from the atomic beam approximately 27 cm downstream from the oven’s nozzle. An approximate beam divergence half-angle of 13 mrad is expected based on the aspect ratio of the nozzle in the molecular flow limit.

After exiting the nozzle, the atoms are transversely cooled with a 2D optical molasses formed by two or-
thogonal laser beams each making about 10 passes across the atomic beam. The atomic beam then passes through a conductance-limiting tube with diameter 2.5 cm and length 1 cm, see Fig. 2. Subsequently, the atoms enter a 1 m long constant deceleration Zeeman slower. Here, we use a $\sigma^+$ slower configuration where the magnetic field decreases with distance as the atoms are slowed. This type of slower is appropriate for the weak transition available in Ra because it allows the slowing region to extend all the way to the magneto-optical trap (MOT). Moreover, the atoms are less affected by transverse heating during the slowing process. The Zeeman slower uses a peak field of 12 G to capture atoms with velocities up to 63 m s$^{-1}$. Finally, we use a three-dimensional MOT to trap the atoms, where a single repump laser beam near 1428 nm and room-temperature blackbody radiation keep the atoms cycling on the cooling transition, see Fig. 1 (left) and Ref. [28].

B. $^{88}$Sr optical trap

The $^{88}$Sr (stable, nat. abd. = 0.83, nuclear spin = 0) system of the optical lattice clock developed at JILA [27] is fully described in Refs. [28–31]. Here we focus only on the $^{88}$Sr source and subsequent atomic beam, transverse cooler, Zeeman slower, and first-stage MOT, see Fig. 3. The atomic beam source is an effusive oven with a cylindrical nozzle of 0.2 cm diameter and 2 cm length. The crucible and nozzle temperatures are 525 °C and 725 °C, respectively. A 0.36 cm diameter filtering aperture located 19 cm downstream of the nozzle provides additional collimation.

After exiting the Zeeman slower, the slowed atoms are captured by a three-dimensional MOT. In the absence of repumping, the cold atoms eventually decay into the metastable “dark” state $^3P_2$, with a 20 ms time constant. According to Ref. [28], the loading rate of the MOT is $2.7(9) \times 10^9$ atoms/s while the atomic flux after the filtering aperture is $3 \times 10^{11}$ atoms/s, which gives the efficiency of the system (excluding the losses due to beam collimation from the filtering aperture) as $\eta_{\text{Sr,exp.}} = 9 \times 10^{-3}$. With two additional lasers to repump the atoms shelved in the long-lived $^3P_2$ state, the MOT lifetime is increased by a factor of 15 and becomes limited by collisions with the residual gas and/or

![FIG. 3. The $^{88}$Sr optical trapping apparatus. Figure from Ref. [31].](image)

All laser-based interactions utilize the electric dipole transition $5s^2 \, ^1S_0 \leftrightarrow 5s5p \, ^1P_1$ near 461 nm, see Fig. 1 (right), with a natural decay rate $\gamma_{\text{Sr}}/2\pi \approx 32$ MHz [23]. The first laser-atom interaction region is a transverse cooling region located shortly after the filtering aperture; this two-dimensional optical molasses is formed by two orthogonal laser beams, each retro-reflected and elliptically shaped to have a long axis in the direction of atomic beam propagation, maximizing the interaction region. Next, the atomic beam passes through a gate valve and a shutter before entering the Zeeman slower. In this case, the slower is operated in a $\sigma^-$ configuration [32], wherein the magnetic field increases with distance as the atom slows. This facilitates a sharp cutoff in the laser-atom interaction as the atom exits the slower. Here, the slower uses a peak magnetic field near 600 G to capture atoms with longitudinal velocities up to about 500 m s$^{-1}$. The Zeeman slower laser beam is assumed to be collimated with an intensity radius ($1/e^2$) of 0.2 cm and a saturation parameter of 12 near the center of the Gaussian beam [27].

| Parameter                             | Units | Sr expt. | Ra expt. |
|---------------------------------------|-------|----------|----------|
| Cooling transition                    |       | $^1S_0 \leftrightarrow ^1P_1$, $^1S_0 \leftrightarrow ^3P_2$ | |
| Transition linewidth $\gamma$         | MHz   | 32       | 0.38     |
| Saturation intensity $I_s$            | mW/cm$^2$ | 41       | 0.14     |
| Transverse cooling intensity $I_s$    | G     | 0.3      | 120      |
| Zeeman slower peak field $G$          |       | 600      | 12       |
| Zeeman slower detuning $\gamma$       |       | 34       | 10       |
| Zeeman slower intensity $I_s$          |       | 12       | 80       |
| MOT laser detuning $\gamma$           |       | 1.3      | 6        |
| MOT beam intensity $I_s$              |       | 0.04     | 11       |
| MOT B-field gradient $G/cm$           |       | 50       | 1        |

TABLE I. Comparison of key parameters in the Sr and Ra experiments. All intensities are given as the peak intensity of the Gaussian beam, before retroreflection, and in units of the saturation intensity. All detunings are given in units of the transition linewidth.

[1] Regarding the beam parameters used in the $^{88}$Sr Zeeman slower, we note [33] that the beam shape is a distorted Gaussian, which when spatially-filtered gave nearly the same slowing efficiency despite having approximately half the total power. Thus we take the effective power as 30 mW.
the $^{88}\text{Sr}$ atomic beam, which passes directly through the MOT. See Tab. I for a summary of the key parameters for both experiments.

III. MONTE CARLO SIMULATION

In order to fully model the optical traps described in Sec. II our MC simulation includes the main optical trapping subsystems (transverse cooler, Zeeman slower, and MOT) and as well as additional experimental details: the atomic beam source, gravity, laboratory magnetic fields, laser frequency noise, and residual gas collisions. We simulate the random walk of individual atoms in gravitational free-fall along the length of the modeled apparatus. The simulation outputs both the complete state of sampled atoms at each time step as well as the collective statistics of an entire simulation run (e.g. the overall trapping efficiency). The following subsections detail our implementation of these subsystems and processes.

A. Modelling the Atomic Beam Source

An effusive oven consists of a crucible and a collimating nozzle. These ovens operate in one of three flow regimes: molecular, intermediate, and viscous. These flow regimes determine the angular intensity and velocity distributions of the output atomic beam. The temperature of the crucible and geometry of the nozzle determine the flow regime of the oven, which is characterized by the Knudsen number,

\[ K_{ns} = \frac{\lambda_{atom}}{d_{noz}} \]  

(short wide nozzle),

\[ K_{nl} = \frac{\lambda_{atom}}{L_{noz}} \]  

(long narrow nozzle),

where $\lambda_{atom}$ is the mean free path of an atom in the oven, see Eq. [1] in appendix [3] and $d_{noz}$ and $L_{noz}$ are the diameter and length of the nozzle, respectively. The aspect ratio of the nozzle,

\[ \chi_{AR} = \frac{d_{noz}}{L_{noz}} \]

characterizes the shape of the nozzle: $\chi_{AR} > 1$ for short wide nozzles and $\chi_{AR} < 1$ for long narrow nozzles. Both the Ra and Sr oven have long narrow nozzles, $\chi_{AR}(\text{Ra}) = 2.4 \times 10^{-2}$ and $\chi_{AR}(\text{Sr}) = 0.1$, and going forward we will refer to the Knudsen number as $K_n \equiv K_{nl}$. For molecular flow ($K_n \gg 1$), the geometry of the nozzle determines the shape of the angular intensity distribution. In the intermediate flow ($K_n \approx 1$) regime, one must account for the influence that both interatomic collisions and the geometry of the nozzle have on the shape of the angular intensity distribution. For viscous flow ($K_n \ll 1$), hydrodynamic effects dominate the shaping of the angular intensity distribution and the total flow rate from the oven. In molecular and intermediate flows, the velocity distribution of effusing atoms is a temperature-dependent Boltzmann distribution, perturbed by a Knudsen-number dependent factor for atoms with trajectories originating from the crucible (as opposed to a nozzle wall). See App. [3] for the formulation of the molecular and intermediate flow regime distributions; we do not consider viscous flow in the simulation.

We generate the angular intensity and velocity distributions from the geometry, temperature, and Knudsen number of the effusive oven in the optical trapping system we are modeling (e.g. the two optical traps described in Sec. II). A single atom is randomly placed within the area of the exit of the nozzle, and its trajectory is randomly sampled from the appropriate angular intensity distribution. We then project this trajectory backwards into the nozzle and crucible to determine the last wall with which the atom last came in contact. We assume the atom reaches thermal equilibrium before leaving this wall, so that the temperature of this wall sets the Boltzmann distribution from which we randomly sample the atom’s velocity. Considering the crucible and nozzle temperatures separately allows simulation of temperature gradients in the oven.

B. Modeling Laser-Atom Interactions

The simulation models each laser field as a composition of circularly and linearly polarized laser beams. Each of these beams is defined by a reference point, propagation direction, transverse elliptical size, Gaussian intensity profile, divergence angle, polarization helicity, saturation intensity, and frequency detuning. We define two types of laser beams in the simulation: transition and repump beams. Each of these beams compete for the excitation of simulated atoms.

The transition beams operate on a defined atomic transition, which we treat as a two-level system with hyperfine splitting. We treat laser-atoms interactions semiclassically in the simulation: photon absorption and spontaneous emission follow electric dipole selection rules and angular distributions, and generate velocity kicks to the atom. Atoms reside in quantum states described by the total electronic angular momentum plus nuclear spin quantum number $F$ and its projection $m_F$ along the quantized axis, which we set along the direction of the external B-field. We assume that both $F$ and $m_F$ are conserved during ballistic flight and that stimulated emission is negligible. The total photon absorption rate is calculated by first determining the Zeeman shift of the $m_F$ states caused by the local magnetic field, see Sec. III C below, and then summing over the Doppler-shift dependent saturation intensity of each beam. We take the photon absorption rate of any one laser beam as the total absorption rate weighted by the fractional saturation intensity contributed by that beam. See App. A for further details on the formulation of these rates.
We also include a stochastic noise process for transition beams such that the central frequency of a beam can undergo a random walk before being damped back to the central value. The noise is specified by an amplitude $\sigma$ and damping time $\tau$. The physical significance of the damping time can be, for example, a laser frequency servo loop with finite bandwidth, which in the Ra optical trap gives a damping time of $\tau = 50\,\mu$s. The corresponding spectral density at each Fourier frequency $f$ is white from D.C. to $f = 0.5/\tau$, after which it falls off like $1/f$.

We treat the repump beams and dark states more simply. Atoms in the excited state can decay to a metastable dark state. We model these dark states with a transition probability from the excited state and a characteristic lifetime that an atom will remain in the dark state. Multiple dark states are treated cumulatively and modeled as a single dark state with an overall transition probability and characteristic lifetime. If an atom is in a dark state and within the defined bounds of a repump laser beam, we return the atom to the ground state after a randomly-selected lifetime-weighted time step.

**C. Magnetic Fields**

Magnetic fields play a key role in modeling subsystems of an optical trapping apparatus, specifically the Zeeman slower and MOT. We include magnetic fields in the simulation from multiple sources: circular coil windings with specified current, ambient field maps, constant background fields, and a two-dimensional axisymmetric Zeeman slower. From these we calculate the total magnetic field as a three-dimensional grid of magnetic field vectors. The value of the local magnetic field is found by interpolating between points on this grid.

**D. Collisions With Residual Gas Molecules**

We consider the effect of collisions with residual gas molecules to simulate how a non-zero vacuum pressure alters an atom’s trajectory in the simulation. Due to shallow trap depths, long-range dispersion forces in the form of induced dipole-dipole force $V = -C_6/R^6$ dominate the collisional cross section for ejection from a MOT, where $C_6$ is the long-range van der Waals coefficient and $R$ is the intermolecular distance. To determine the collision frequency, scattering angle, and outgoing velocity, we first calculate the mean free path of the atom based on kinetic theory, from which we randomly determine the distance the atom travels before a collision. When a collision event occurs, we randomly sample the velocity of the residual gas molecule from a room-temperature Boltzmann distribution, and an impact parameter from a uniform distribution. Collisions with impact parameters beyond a specified cutoff value are ignored as we assume these lack the energy to significantly alter an atom’s trajectory. With these values, and specified $C_6$ coefficients and interaction distances, we numerically calculate the Lennard-Jones dynamics to find the scattering angle and outgoing velocity, and update the atom’s trajectory accordingly.

**E. Simulating An Atom’s Random Walk**

We begin the simulation by generating an atom at the source oven as described in Sec. III A, see Fig. 4 (left). The atom will then proceed in a random walk through a series of time steps chosen based on the photon scattering and residual gas collision rates. All time steps are clamped to a specified maximum value. At the start of a time step, we calculate the photon absorption, spontaneous emission, repumping, and residual gas collision rates. Based on these rates, the shortest time step until the next event is chosen. We then update the atom’s position and velocity accordingly while holding these rates constant. At the end of the time step, the process indicated by the rate the time step is chosen from is performed, and then a new iteration is started. We continue tracking an atom through these time steps until one of the following scenarios occur: the atom encounters a physical barrier (such as an aperture), leaves the defined bounds of the simulation, exceeds the specified total time limit, or becomes trapped in the MOT, see Fig. 4 (right). Finally, we terminate the simulation of that atom and update the lost and trapped atom counts accordingly.

**F. Numerical Implementation**

The simulation code consists of modules written in Fortran 90 and C, and we utilize the CERNLIB Programming Library for numerical calculations. In order to parallelize our code, we use the Master/Slave algorithm implemented by the Asynchronous Dynamic Load Balancing (ADLB) Fortran interface to Message Passing Interface standard. Using ADLB allows for work-sharing among a number of processors and computer nodes in a distributed-memory system. This permits rapid investigation of a large number of parameters.
that affect the efficiency of the simulated optical traps.

IV. COMPARISON TO EXPERIMENT

In order to accurately model each of the optical traps described in Sec. II, we include all laser beams, known magnetic fields, and geometry using experimentally determined parameters. For each simulation, initial velocity and angular cuts discard atoms with velocity vectors that immediately leave the simulation bounds upon exiting the oven and atoms that have an initial velocity exceeding what the Zeeman slower can sufficiently slow. We minimize statistical errors in the simulation by simulating several thousand atoms within these angular and velocity cuts. In the Ra experiment we define the total efficiency as the ratio of the number of atoms trapped to the number of atoms exiting the source oven, as obtained by fluorescence measurements of the MOT and atomic beam, see Fig. 2. The $^{88}$Sr efficiency definition differs in that the number of trapped atoms is compared to the number of atoms passing through the filtering aperture, not the total number exiting the oven.

We determine the simulated optical trapping efficiency in the same manner as the experimental value. The fluorescence measurements rely on limited knowledge of scattering rates, detector efficiencies, and detector solid angles, which results in roughly a factor of 3 uncertainty in the experimentally-determined trap efficiencies. We expect that ratios of experimentally-determined trapping rates, detector efficiencies, and detector solid angles are not the total number exiting the source oven.

For the $^{88}$Sr simulation, we use the experimental slowing beam parameters, see Sec. II B and Tab. II, and find a $^{88}$Sr optical trapping efficiency of $\eta_{\text{Sr,sim}} = 4 \times 10^{-3}$. By adding transverse cooling, we see a four-fold increase in efficiency to $\eta_{\text{Sr,sim}} = 1.6 \times 10^{-2}$, which is in within a factor of 3 to the experimental value of $\eta_{\text{Sr,exp}} = 0.9 \times 10^{-2}$. Additionally, we find the trapping efficiency strongly depends on the slowing beam size and intensity. We observe that for a fixed optical power, we achieve optimal slowing using a central intensity of $4I_s$, and that increasing the beam size while maintaining this central intensity leads to higher trapping efficiency due to better overlap between the atomic and slowing laser beams. By expanding the slowing beam’s intensity radius ($1/e^2$) to 0.4 cm, we further increase in the $^{88}$Sr optical trapping efficiency by another factor of about 4.

For the $^{225}$Ra simulation, we find a baseline optical trapping efficiency from slowing of the atomic beam of $\eta_{\text{Ra,sim}} = 4 \times 10^{-7}$. With the addition of both transverse cooling and repumping of the atomic beam, we find gains in efficiency of approximately 60 and 2.4, respectively, increasing the efficiency to $\eta_{\text{Ra,sim}} = 5.7 \times 10^{-5}$. This disagrees with the experimental value of $\eta_{\text{Ra,exp}} = 2 \times 10^{-6}$ by a factor of 30. Despite this discrepancy between the experimental and simulated total optical trapping efficiencies, we note the relatively good agreement on gain in efficiency produced by inclusion of the the transverse cooling region and the 1428 nm repump laser (co-propagating with the slower laser). See Tab. II for a comparison of the experimental and simulated optical trapping efficiencies in the $^{88}$Sr and $^{225}$Ra optical traps.

TABLE II. Comparison of $^{88}$Sr and $^{225}$Ra optical trapping efficiencies from experiment and simulation. ($\eta$: trapping efficiency; ZS: Zeeman slower; TC: transverse cooling) The systematic uncertainty in the experimentally determined total efficiencies is about a factor of 3. The statistical uncertainty in the simulated total efficiencies is about 5%.

|                     | $^{88}$Sr exp. | $^{88}$Sr sim. | $^{225}$Ra exp. | $^{225}$Ra sim. |
|---------------------|---------------|----------------|-----------------|-----------------|
| $\eta_{\text{ZS only}}$ | $2 \times 10^{-3}$ | $4 \times 10^{-3}$ | $1 \times 10^{-8}$ | $4 \times 10^{-7}$ |
| TC gain             | 4             | 4              | 60              | 60              |
| Repump gain         | n/a           | n/a            | 3.5             | 2.4             |
| $\eta_{\text{total}}$ | $9 \times 10^{-3}$ | $1.6 \times 10^{-2}$ | $2 \times 10^{-6}$ | $5.7 \times 10^{-5}$ |

V. SENSITIVITY STUDIES OF THE RADIUM OPTICAL TRAP

To diagnose the source of the discrepancy between the simulated and measured values of the $^{225}$Ra optical trapping efficiency, we simulate possible systematic effects in the experiment that we did not originally account for in the simulation. The simulation's accurate prediction of relative gains in optical trapping efficiency allows for sensitivity studies to quantify the extent to which these systematic effects contribute to a reduced efficiency.

A. Influence of Residual Gas Inside the Oven

In both the experiment and simulation, we assume that the dominant factor determining the mean free path of Ra is the saturated vapor pressure of Ba in the oven; all other known materials in the oven have vapor pressures significantly lower than Ba at the 500°C operating temperature (SVP$_{Ba}$ = 138 μTorr). This gives a mean free path of $\lambda_{Ra} \approx 42$ cm and Knudsen number $K_n \approx 5.1$, so we assume the oven operates in the intermediate flow regime. Any additional constituents within the oven with comparable (or higher) vapor pressures than Ba will reduce $\lambda_{Ra}$ and broaden the angular distribution of the atomic beam exiting the oven. We fabricate the oven’s crucible from Ti, which can absorb and store a significant amount of H$_2$ [39], so we cannot rule out the possibility that there is a significant H$_2$ partial pressure.

To characterize the impact that an increased H$_2$ partial pressure in the oven has on the optical trapping efficiency, we simulate a varying oven angular distribution by varying its Knudsen number from the oven’s $K_n \approx 5.1$ down to the intermediate/viscous flow regime boundary at $K_n = \chi_{AR} = 2.4 \times 10^{-2}$. We do not consider the vis-
cous flow regime in our simulation. From the results of these simulations, see Fig. 5, we find that it takes a $\text{H}_2$ partial pressure in the oven $>1 \times 10^{-3}$ Torr ($K_n \approx 1$) to see a significant decrease in the optical trapping efficiency below our initial results using only Ba to determine the oven’s angular distribution. For $\text{H}_2$ in the oven to significantly contribute to the discrepancy between measured and simulated trapping efficiencies, a partial pressure $\gg 2$ mTorr is required, which may be possible due to differential pumping given the conductance of the oven nozzle. Without means to directly measure the pressure in the oven, we cannot rule out the influence of residual gas inside the oven as a contribution to the discrepancy between the measured and simulated optical trapping efficiencies.

FIG. 5. The influence of $\text{H}_2$ partial pressure in the oven on the optical trapping efficiency. Data points represent a varying $\text{H}_2$ partial pressure and a constant Ba partial pressure of 138 $\mu$Torr at an oven temperature of 500 °C. The optical trapping efficiency remains unchanged until reaching a $\text{H}_2$ partial pressure of about $3 \times 10^{-4}$ Torr, approximately a Knudsen number of $K_n \approx 2$ which is well within the bounds of the intermediate flow regime.

B. Misaligned Oven Nozzle

A misalignment between the oven nozzle and Zeeman slower axis potentially reduces the optical trapping efficiency. We can partially correct for this in the experiment by carefully realigning the transverse cooling beams. To model these misalignments in the simulation, we rotate and translate the oven nozzle off the Zeeman slower axis. From mechanical constraints, we bound these misalignments to $\pm 10^\circ$ and $\pm 1$ cm, respectively. For these studies we do not modify the properties of the transverse cooler to correct for the induced misalignments. The results, see Fig. 6, show that small misalignments of the nozzle do not alone cause the factor of 30 discrepancy in trapping efficiency with the experimental results, although we cannot rule out a small contribution.

FIG. 6. Simulated optical trapping efficiency with oven nozzle misalignments. Rotations and offsets are in the XZ-plane where the Zeeman slower is aligned along the Z-axis.

C. Influence of Residual Gas Outside the Oven

To test the effect of a non-zero vacuum pressure in the transverse cooling region, we simulate collisions between Ra and a residual gas of $\text{H}_2$. With estimates for the $C_6$ coefficients and bond lengths as described in App. C, we find that our baseline vacuum pressure ($3 \times 10^{-7}$ Torr) reduces the $^{225}\text{Ra}$ optical trapping efficiency by a factor of 1.4 when compared to the collision-free scenario. Increasing the pressure in the transverse cooling region by a factor of 10 further reduces the efficiency by a factor of 1.9, see Fig. 7. These results suggest that the $^{225}\text{Ra}$ optical trapping efficiency is only weakly sensitive to residual gas collisions in the transverse cooling region, which may indicate that low impact collisions can be corrected for with optical forces. We also simulated the MOT with our residual gas collision model and determined a MOT trap lifetime of 15 s which agrees with the experimentally determined value at a residual gas pressure of $10^{-9}$ Torr to better than a factor of two.

D. Stray Magnetic Fields in the Transverse Cooler

We include all known magnetic sources in the simulation, including the Zeeman slower, MOT coils, and the uniform contribution from the earth’s magnetic field as measured in the laboratory. We do not explicitly include stray magnetic fields, such as those from ion pump magnets and high current heating elements in the oven. In order to test the effect that these stray fields have on the trapping efficiency, we model magnetic fields in the transverse cooling region by adding fictitious coils and varying their orientation and magnetic strength. The results of these simulations, see Fig. 8, show that a stray magnetic field of magnitude in excess of 1 G is required to significantly reduce the optical trapping efficiency to
FIG. 7. The influence of vacuum pressure in the transverse cooling region on the optical trapping efficiency. Data points represent a varying $\text{H}_2$ number density at room temperature.

the levels measured in the apparatus. Furthermore, in order to test the predictions of the simulation results, we added rectangular coils in the TC region and experimentally measured the change in the atomic fluorescence from the MOT as a function of applied magnetic field in the TC region using $^{226}\text{Ra}$ as a surrogate for $^{225}\text{Ra}$. The measured results qualitatively agree with the simulation, namely a stray field of in excess of 1 G is needed to significantly lower the trapping efficiency. We do not expect uncontrolled fields of this magnitude within the Ra optical trap so we do not expect these stray magnetic fields to be a major contributor to the discrepancy between the measured and simulated optical trapping efficiencies.

E. Laser Frequency Noise

In the Ra optical trap, we generate the 714 nm light with a Ti:sapphire ring laser referenced to a high-finesse optical cavity. The resulting laser spectrum is mostly white with a few peaks in the kHz range, and we measure the overall linewidth to be approximately $100 \text{kHz} \approx 0.3 \gamma_{\text{Ra}}$. We simulate potential noise sources by varying the noise amplitude and damping time associated with individual laser beams. Based on the results of these simulations, see Fig. 9, we do not expect the $^{225}\text{Ra}$ optical trapping efficiency to be limited by laser linewidth and frequency noise.

F. MOT Beam Misalignment and Imbalance

We trap Ra atoms using a 3D MOT created by a quadrupole magnet and three orthogonal laser beams of the appropriate helicity intersecting where the magnetic field goes to zero. These beams are retroreflected outside of the vacuum chamber. We measured the optical losses due to reflections from the vacuum viewports and found that the retroreflected beams have 10% less power than their forward-going counterparts. These six laser beams are modelled as three intensity-imbalanced orthogonal pairs of anti-parallel and opposite helicity beams. In the simulation, this imbalance produces a small shift in the position of the MOT’s center, but no change in the trapping efficiency is observed. Further increases to the intensity imbalance between pairs of retroreflected beams

FIG. 8. The influence of stray magnetic fields on the $^{226}\text{Ra}$ optical trapping efficiency. Fields are simulated with coil windings placed along each of the coordinate axes in the transverse cooling region with varying values of current. The shifts in the peak efficiency are, shown in the upper two plots, are due to the Earth’s magnetic field in the simulation, which is “tuned out” in the experimental setup. The bottom two plots show the efficiencies when the Earth’s magnetic field is “turned off” in the simulation.

FIG. 9. The influence of laser frequency noise on the $^{225}\text{Ra}$ optical trapping efficiency. The horizontal axis ($\sigma$) is the laser linewidth in terms of the Ra atomic linewidth. The different curves correspond to different values of the damping time $\tau$.
likewise shifted the MOT center while leaving the trapping efficiency unchanged. This agrees with our assumption that the MOT operates at a very high saturation parameter, lessening the effect of small changes in the global intensity on the optical trapping efficiency.

While ensuring anti-parallelism between each MOT beam and its retroreflection is relatively straightforward experimentally, it is more difficult to ensure that the global overlap of the three beams is optimal. We tested the impact of sub-optimal MOT beam overlap in the simulation by individually offsetting one pair of beams from the others. Generally speaking, displacements of up to 1 cm (approximately the intensity radius of the MOT beams) produces no significant losses in the optical trapping efficiency, and we do not expect misalignments in the experiment to be any larger than this.

VI. SUMMARY & CONCLUSIONS

We have presented a three-dimensional MC simulation of an optical trapping apparatus that includes the effects of several common perturbations to the laser cooling and trapping process. With this simulation we model the optical trapping apparatus used in our $^{225}$Ra EDM measurements in an effort to improve our optical trapping efficiency of $^{225}$Ra. Our simulation mostly agrees with the experimental results of both the $^{225}$Ra and $^{88}$Sr optical trapping systems, i.e. we see the same relative gains in trapping efficiency from switching on/off components of the apparatus, and we find good agreement between the measured and simulated $^{88}$Sr optical trapping efficiencies. However, the $^{225}$Ra simulation results differ from experimental results by a factor of 30. We note that we may not see the discrepancy between measured and simulated trapping efficiencies in the $^{88}$Sr optical trap since we do not consider the full trapping efficiency in the system. Simulations of possible systematic effects in the apparatus so far have shown that there is no sole-source of this discrepancy, but rather these effects may cumulatively explain this difference between the measured and simulated trapping efficiencies.

In addition to these systematic effects, potential contributions to this discrepancy may result from other aspects of our simulation. For example, our treatment of the effusive-oven atomic beam source may not be adequate for the complex chemistry in the Ra oven. We plan on determining the adequacy of this atomic beam source model by detailed study of the output of effusive ovens with chemical surrogates for Ra (such as Ca) in comparison to the simulation’s predictions.

While a discrepancy exists between the measured and simulated optical trapping efficiencies, the accurate relative gains predicted by the simulation for both the Ra and $^{88}$Sr optical traps makes this simulation a valuable tool for studying and optimizing the optical trapping of rare isotopes. In the case of the $^{225}$Ra optical trap, we plan to use the simulation to test and optimize and a planned “blue slower” upgrade. Our present “red-slower” scheme ($^3S_0 \leftrightarrow ^3P_1$ near 714 nm) can only slow and trap atoms with initial velocities of up to $63 \text{ m s}^{-1}$, approximately $< 0.5\%$ of the oven’s velocity distribution. The blue-slower upgrade will use the stronger $^1S_0 \leftrightarrow ^1P_1$ transition near 483 nm, allowing us to slow and trap atoms with initial velocities of up to $310 \text{ m s}^{-1}$, approximately 50\% of the oven’s velocity distribution. Implementing this scheme will require frequency chirping of the slowing laser and additional repump lasers to handle the additional atomic dark states associated with this transition. We plan on upgrading the simulation to include both frequency chirping and additional repumping transitions, and using the upgraded simulation to help implement and optimize the blue slower in the $^{225}$Ra optical trap. This upgrade to the $^{225}$Ra optical trap will offer increased EDM measurement precision by increasing our optical trapping efficiency by up to two orders of magnitude.

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Appendix A: Calculation of photon absorption rates

We decompose the laser field into an array of circularly and linearly polarized beams, all of which compete for the excitation of the atom. The beams are described by a reference point $X$, a propagation direction $\vec{p}$, transverse elliptical size $(r_1, r_2)$, Gaussian intensity profile $(\sigma_1, \sigma_2)$, divergence angle $(\theta_1, \theta_2)$, polarization helicity $(h = \pm 1)$ for circularly polarized and $h = 0$ for linearly polarized), saturation intensity $I = I/\text{sat}$ and detuning $\Gamma = \delta/\gamma_{R_a}$ is the detuning. Evaluating the integral we find

$$\beta = \beta_0 \int_{-\infty}^{\infty} \frac{L(x) dx}{1 + 4(x + \Gamma)^2}$$  \hspace{1cm} (A6)

where $\beta_0 = I/I_{\text{sat}}$ is the on-resonance saturation parameter, $L(x)$ is a normalized Lorentzian function, and $\Gamma = \delta/\gamma_{R_a}$ is the detuning. The beams are described by $h$ for circularly polarized and $\theta$ for linearly polarized.

We determine the intensity $\beta_i$ and photon direction $\vec{p}_i$ of each beam (indicated by the subscript $i$) at the location of the atom. The Zeeman shift of the upper (lower) state in natural linewidths per unit $m_F$ is $[40]$

$$Z_{i(u)} = \frac{\mu_B g_{i(u)}}{\hbar} B \tau$$  \hspace{1cm} (A1)

where $\mu_B$ is the Bohr magneton and $\hbar$ the reduced Planck constant, $g_{i(u)}$ is the Landé g-factor of the upper (lower) state, $\tau$ is the natural lifetime of the upper state, and $B \equiv |\vec{B}|$ is the magnetic field amplitude.

The angular distribution for the transition probability $[40]$ $W_{i,\Delta m}$ for circularly polarized light $(h = \pm 1)$ is:

$$W_{i,1} = \frac{1}{4} (1 + h \cos (\theta_i))^2$$

$$W_{i,0} = \frac{1}{2} \sin^2 (\theta_i)$$

$$W_{i,-1} = \frac{1}{2} (1 - h \cos (\theta_i))^2$$  \hspace{1cm} (A3)

and for linearly polarized light $(h = 0)$ by:

$$W_{i,1} = \frac{1}{2} \cos^2 (\theta_i)$$

$$W_{i,0} = \sin^2 (\theta_i)$$

$$W_{i,-1} = \frac{1}{2} \cos^2 (\theta_i)$$  \hspace{1cm} (A4)

where $\theta_i$ is the angle between $\vec{B}$ and $\vec{p}_i$, and $\Delta m = 0, \pm 1$ is the change in $m_F$ for the transition. We treat all linear polarization as vertical since there is no preferred direction orthogonal to $\vec{p}_i$ in the frame of the laser beam. We sum over the contributions of $W_{i,\Delta m}$ to find the effective intensity of each laser $i$:

$$\beta_i' = \sum_{\Delta m = -1}^{1} \beta_i^{\prime}_{\Delta m}$$

$$= \frac{\beta W_{i,\Delta m}}{1 + 4 |\Gamma_i + D_i + m_F Z_i - (m_F + \Delta m) Z_i|^2}$$  \hspace{1cm} (A5)

We model a non-zero laser linewidth by re-defining the saturation parameter $\beta$ as

$$\beta = \beta_0 \int_{-\infty}^{\infty} \frac{L(x) dx}{1 + 4(x + \Gamma)^2}$$  \hspace{1cm} (A6)

where $\beta_0 = I/I_{\text{sat}}$ is the on-resonance saturation parameter, $L(x)$ is a normalized Lorentzian function, and $\Gamma = \delta/\gamma_{R_a}$ is the detuning. Evaluating the integral we find

$$\frac{\beta}{\beta_0} = \frac{1 + w}{4\Gamma^2 + (1 + w)^2}$$  \hspace{1cm} (A7)

where $w$ is the full-width at half-maximum of the Lorentzian. In the limit $w \to 0$, we recover the familiar definition of the saturation parameter $[41]$. This effectivensilc absorption spectrum, leading to increased excitation probability at large detuning, but reduced excitation probability close to resonance.

The total absorption rate ($R_T$) and fractional absorption rate ($R_{i,\Delta m}$) for each beam $i$ are:

$$R_T = \frac{\beta_T'}{2(2 + \beta_T') \tau}$$

$$R_{i,\Delta m} = R_T \left( \frac{\beta_{i,\Delta m}'}{\beta_T'} \right)$$  \hspace{1cm} (A8)

where $\beta_{i,\Delta m}' = \sum_i \beta_{i,\Delta m}'$ is the total intensity. We emphasize that this is the photon absorption rate for the ground state of the atom; once the atom is excited, we set the absorption rate to zero and the emission rate to $\gamma$, ignoring stimulated emission.

Appendix B: Effusive oven velocity and angular distributions

For an an effusive oven with a Knudsen number $K_n = \lambda_{\text{atom}}/L_{\text{nozzle}}$, we calculate the mean free path of the atom:

$$\lambda_{\text{atom}} = \frac{k_B T}{\sqrt{2\pi d^2 P}}$$  \hspace{1cm} (B1)

where $k_B$ is the Boltzmann constant, $T$ is the temperature, $d$ is the interaction distance between two atoms (taken as the sum of the van der Waals radii), and $P$ is the saturated vapor pressure at a temperature $T$, calculated as $[42]$:

$$\log_{10} \left( \frac{P}{X} \right) = A + \frac{B}{T} + C \log_{10} T + \frac{D}{T^2}$$  \hspace{1cm} (B2)

where $X$ is the pressure per atmosphere in the desired units, and $A, B, C, D$ are experimentally obtained coefficients available in Ref. $[42]$.

We determine the velocity distribution of the atoms in the simulation by the temperature $T$ of the last wall in the oven or nozzle that an atom collides with as $[43–45]$:

$$f(u) = A[f_{\text{beam}}(u)P(K_n, \psi(u))]$$  \hspace{1cm} (B3)
where \( u \) is the reduced velocity \( v_z / \bar{v} \) (\( v_z \) is the longitudinal component of the velocity) and \( \delta \equiv \sqrt{2K_B T/M} \) is the most probable velocity where \( M \) the mass of the atom. \( A \) is a normalization constant satisfying \( \int_0^\infty f(u) \, du = 1 \). The unperturbed Boltzmann distribution for an atomic beam is:

\[
f_{\text{beam}}(u) = \frac{2u^3}{\bar{v}} \exp \left( -u^2 \right)
\]

and the Knudsen number perturbation is:

\[
P(K_n, \psi(u)) = \frac{\sqrt{\pi} \operatorname{erf}(\psi(u)/2K_n)}{\sqrt{\psi(u)/2K_n}} \quad \text{(B5)}
\]

with the function \( \psi(u) \) defined as:

\[
\psi(u) = \frac{ue^{-u^2} + (\sqrt{\pi}/2)(1 + 2u^2) \operatorname{erf}(u)}{\sqrt{2\pi}u^2} \quad \text{(B6)}
\]

We include both the molecular and intermediate flow regime distributions in the simulation and reproduce the formulas from Refs. 13 and 14 below. The molecular flow angular distribution depends solely on the oven nozzle’s geometry, and for polar angles \( \theta \) from the axis of the atomic beam, the distribution of angles originating from the oven \( \chi_{\text{AR}} \geq \tan \theta \) where \( \chi_{\text{AR}} = d_{\text{noz}}/L_{\text{noz}} \) is:

\[
j_M(\theta) = \zeta_0 \cos \theta + \frac{2}{\pi}[(1 - \zeta_0)R(q)] \cos \theta + \frac{4}{3\pi q} \left[ 1 - (1 - q^2)^{3/2} \right] \zeta_1 - \zeta_0 \cos \theta \quad \text{(B7)}
\]

and for angles originating from the nozzle wall \( \chi_{\text{AR}} \leq \tan \theta \):

\[
j_M(\theta) = \zeta_0 \cos \theta + \frac{4}{3\pi q} \zeta_1 - \zeta_0 \cos \theta \quad \text{(B8)}
\]

where the following definitions are used:

\[
q = \tan \theta / \chi_{\text{AR}} \quad \text{(B9)}
\]

\[
R(q) = \cos^{-1}(q) - q\sqrt{1 - q^2} \quad \text{(B10)}
\]

and the collision rates with the nozzle walls at the exit and entrance, \( \zeta_0 \) and \( \zeta_1 \), respectively, are two dimensionless parameters defined as:

\[
\zeta_0 = \zeta_1 - \frac{(1 + 2/\chi_{\text{AR}})\sqrt{1 + 1/\chi_{\text{AR}}^2} - (1 + 2/\chi_{\text{AR}})}{\sqrt{1 + 1/\chi_{\text{AR}}^2} + 1}
\]

\[
\zeta_1 = [1 + \chi_{\text{AR}}/(2 + \chi_{\text{AR}}^2)]^{-1} \quad \text{(B11)}
\]

The intermediate flow regime angular distribution accounts for both the nozzle’s geometry and interatomic collisions in the nozzle. This distribution depends on the Knudsen number as well as the number density of the atoms at the exit and entrance of the nozzle, characterized by the two dimensionless parameters \( \xi_0 \) and \( \xi_1 \), which are conventionally defined as \( \xi_0 \equiv \zeta_0 \) and \( \xi_1 \equiv \zeta_1 \). The distribution for \( \chi_{\text{AR}} \geq \tan \theta \) is:

\[
j_M(\theta) = \xi_0 \cos \theta \left[ 1 + \frac{2}{\sqrt{\pi}} \frac{e^{\xi_0^2}}{\delta} S(q) \right] + \frac{\xi_0 \cos \theta e^{\xi_0^2}}{\sqrt{\pi}} \left[ R(q) \left( \operatorname{erf}(\xi' - \operatorname{erf} \delta + F(\xi_0, \xi_1, \delta')) \right) \right] \quad \text{(B12)}
\]

and for \( \chi_{\text{AR}} \leq \tan \theta \):

\[
j_M(\theta) = \xi_0 \cos \theta \left[ 1 + \frac{2}{\sqrt{\pi}} \frac{e^{\xi_0^2}}{\delta} S(1) \right] \quad \text{(B13)}
\]

and at \( \theta = 0 \):

\[
j_M(0) = \xi_0 + \frac{\sqrt{\pi}}{2} \xi_0 e^{\xi_0^2} \left( \operatorname{erf} \xi - \operatorname{erf} \delta \right) + \frac{(1 - \xi_1)}{\xi_0} e^{-(\xi^2 - \delta^2)} \quad \text{(B14)}
\]

where the following definitions are used:

\[
\delta = \sqrt{\frac{\xi_0^2}{2K_n(\xi_1 - \xi_0)}} \quad \xi = \left( \frac{\xi_1}{\xi_0} \right) \delta \quad \text{(B15)}
\]

\[
\delta' = \sqrt{\frac{\delta^2}{\cos \theta}} \quad \xi' = \left( \frac{\xi_1}{\xi_0} \right) \delta' \quad \text{(B16)}
\]

\[
F(\xi_0, \xi_1, \delta') = \frac{2}{\sqrt{\xi_0^2}} \xi' \left( \frac{1}{\xi_1} - 1 \right) e^{-\xi^2} \quad \text{(B17)}
\]

\[
S(q) = \int_0^q dz \sqrt{1 - z^2} \times \left( \operatorname{erf} \left( \delta' \left[ 1 + z \left( \frac{\xi_1}{\xi_0} - 1 \right) \right] \right) - \operatorname{erf} \delta' \right) \quad \text{(B18)}
\]

**Appendix C: Estimate of long-range van der Waals \( C_6 \) coefficients**

Residual gas collisions alter an atom’s trajectory and can eject atoms from the MOT. To assess the impact of these effects on the optical trapping efficiency, we included a non-zero residual gas pressure in the simulation. For relevant residual gases in the \(^{225}\)Ra optical trap, e.g. \( \text{H}_2 \) and \( \text{Ar} \), no data exists for the \( C_6 \) coefficient with \( \text{Ra} \). Instead, we estimate the coefficients with the London dispersion formula:

\[
C_6 = \frac{3}{2} \left( \frac{U_1U_2}{U_1 + U_2} \right) \alpha_1 \alpha_2 \quad \text{(C1)}
\]
where \( \alpha_i \) is the polarizability (in \( \text{Å}^3 \)) and \( U_i \) a relevant energy scale for each constituent. For tightly bound species such as molecules and noble gases, we estimate \( U_i \) as the ionization energy, whereas for alkaline earths, such as Ra and Ba, we estimate \( U_i \) as the energy of the \( ^1S_0 \rightarrow ^1P_1 \) transition, as this state dominates the ground state polarizability. We then calculate a table of \( C_6 \) coefficients from this estimate, which agree to within 10% with accepted values, see Tab. III. Since the total scattering cross section scales as \( (C_6)^{1/3} \) \cite{46}, calculations of collisional processes are only weakly sensitive to small errors in this coefficient. We also require a bond length to generate a Lennard-Jones potential for each pair of objects. In the case of the \(^{225}\text{Ra}\) simulation, we estimate this by adding the atomic radius of Ra (2.15 Å) to the effective radius of the other object. While not precise, in these simulations the final results are insensitive to the exact details of the short-range interaction since such a low impact parameter collision is certain to alter the trajectory and/or eject the \(^{225}\text{Ra}\) atom from the MOT.

|       | Ra  | Ba  | \( \text{H}_2 \) | Ar  |
|-------|-----|-----|------------------|-----|
| \( U (\text{eV}) \) | 2.57 | 2.53 | 15.43            | 15.76 |
| \( \alpha (\text{Å}^3) \) | 37.9 | 39.7 | 0.8042           | 1.63  |
| Ra    | 2770 | 2870 | 101              | 205  |
|       | \( 3042 \) \cite{47} | \( 3110 \) \cite{48} | \( 104 \) | \( 211 \) |
| Ba    | 2980 |       | 104              | 211  |
|       | \( 3110 \) \cite{48} |       | \( 104 \) | \( 211 \) |
| \( \text{H}_2 \) |       |       | 7.48             | 15.3 |
|       |       |       | \( 7.29 \) \cite{49} | \( 16.6 \) \cite{50} |
| Ar    |       |       | 31.3             |       |
|       |       |       | \( 34.8 \) \cite{51} |       |

TABLE III. Table of \( C_6 \) coefficients calculated using the London dispersion formula. All entries are in \( \text{eV Å}^6 \). Accepted values listed in italics and are in agreement with our estimated values to within 10%. The values for \( \text{H}_2 \) are for its vibrational ground state.