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Precise Quantum Measurement of Vacuum with Cold Atoms

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We describe the cold-atom vacuum standards (CAVS) under development at the National Institute of Standards and Technology. The CAVS measures pressure in the ultra-high and extreme-high vacuum regimes by measuring the loss rate of sub-millikelvin sensor atoms from a magnetic trap. *Ab-initio* quantum scattering calculations of cross sections and rate coefficients relate the density of background gas molecules or atoms to the loss rate of ultra-cold sensor atoms. The resulting measurement of pressure through the ideal gas law is traceable to the second and the kelvin, making it a primary realization of the pascal. At NIST, two versions of the CAVS have been constructed: a laboratory standard used to achieve the lowest possible uncertainties and pressures, and a portable version that is a potential replacement for the Bayard-Alpert ionization gauge. Both types of CAVSs are connected to a combined extreme-high vacuum flowmeter and dynamic expansion system to enable sensing of a known pressure of gas. In the near future, we anticipate being able to compare the laboratory scale CAVS, the portable CAVS, and the flowmeter/dynamic expansion system to validate the operation of the CAVS as both a standard and vacuum gauge.

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I. INTRODUCTION

As a National Metrology Institute, the National Institute of Standards and Technology (NIST) is tasked with

43 creating primary measurement standards that realize the International System of Units (SI). NIST is especially in-

terested in developing quantum SI standards, i.e. those based on fundamental physical constants and laws. For pressure measurements in high vacuum, ultra-high vacuum (UHV) or extreme-high vacuum (XHV), this could rely on the equation of state $p = \rho kT$ for an ideal gas in thermal equilibrium, where determining pressure p is reduced to determining number density ρ and temperature T. Here, the Boltzmann constant k is exactly defined in the SI. To date, however, *in situ* commercial vacuum sensors that operate below 1×10^{-4} Pa,^{1,2} covering the entire UHV and into the XHV regimes,^{3,4} must be calibrated in order to make SI traceable measurements⁵ and have limited use as transfer standards due to instability or being operated in non-ideal environments.

Much of today's advanced manufacturing and research relies on the availability of ultra-high and extremehigh vacuum. Applications include the characterization of space-simulation chambers and instruments intended for space-flight,^{6,7} the calibration of mass spectrometers,⁸ extreme ultra-violet lithography,⁹ molecular beam epitaxy,^{10,11} scanning electron microscopes, and various techniques for the investigation of surfaces and thin films such as x-ray photoelectron spectroscopy, auger electron spectroscopy, and secondary ion mass spectrometry.^{12,13} Accelerator facilities, synchrotrons, and gravitational wave observatories operate in the UHV and XHV.¹⁴ Moreover, equipment attached to these devices can require UHV environments. Polarized electron sources, for example, rely on photocathodes that have lifetimes limited by ion back-bombardment from residual gas in the environment.¹⁵ Of particular interest to NIST are quantum sensing and quantum computing applications, such as those that utilize cold-atom and trappedion technologies, where obtaining UHV conditions is critical for maintaining entanglement and coherent operation. All applications rely on gauges and mass spectrometers for the determination of the vacuum pressure.

Standards for pressures below 10^{-4} Pa are commonly based on the dynamic expansion technique that requires a flow standard and an expansion chamber with large vacuum pumps. The lower pressure limit of these devices is generally determined by outgassing, pumping speed, and the ability to produce low gas-flows; these constraints limit most systems to pressures above 10^{-7} Pa, but some have obtained ultimate generated pressures on the order of 10^{-10} Pa.^{16,17} These source-based calibration devices are traceable to calibrated pressure gauges operating at pressures above 1 Pa. They occupy several cubic meters of space and require extensive resources to operate, which makes them impractical for *in situ* calibration of gauges or mass spectrometers in most industrial or research environments. Dynamic expansion devices, however, are commonly used by National Metrology Institutes and secondary calibration laboratories for the calibration of gauges.^{16,18–21}

To replace dynamic expansion standards, NIST re-

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cently launched a program to develop a novel, compact quantum-SI standard for vacuum, the cold-atom vacuum standard (CAVS), which utilizes the measured lifetime of trapped neutral atoms with a temperature less than 1 mK to determine the pressure of the background gas. As early as the 1980s, soon after the first successful laser cooling and trapping experiments with neutral alkali-metal atoms, researchers realized that residual room-temperature background gases in thermal equilibrium with the walls of their vacuum chambers limit the lifetime τ of the atoms in their trap (the "trap lifetime"). Early estimates of these background-collisioninduced lifetimes are on the order of 100 s for a background pressure of 1×10^{-8} Pa.²² Several research groups have "inverted" the problem to propose and later to use the trap lifetime as a measurement of pressure in the vacuum chamber.^{23–29} We use either Li or Rb alkali-metal isotopes as sensor

atoms in the CAVS. Lithium is the lightest of the alkalimetals and thus easiest to eject from a trap. It also has the advantage of a negligible vapor pressure near room temperature. Rubidium, however, has the advantage of requiring relatively inexpensive lasers for trapping and cooling. In addition, Rb is easier to trap compared to Li owing to the unresolved hyperfine structure of the relevant electronic excited state of Li. Sub-millikelvin sensor atoms are ejected from the CAVS with near 100% efficiency by collisions with the residual room-temperature atoms and molecules as the imparted momentum or final kinetic energy of the sensor atom is easily larger than the potential energy or depth of the shallow traps with which these atoms are confined. Our atoms are trapped due to the coupling of a non-zero magnetic moment with a static, spatially dependent magnetic field. For typical sensor-atom temperatures, the trap localizes the atoms in a volume significantly below one cubiccentimeter where the field strength has a minimum. Now, as atom-trap depths are typically less than ten times the energy equivalent of the sensor-atom temperature, collisions with room-temperature atoms and molecules easily impart sufficient momentum to the sensor atom.

The number of sensor atoms has an exponential time dependence with decay rate Γ proportional to the number density ρ of the residual gas. In fact, $\rho = \Gamma/L$, where L is the loss-rate coefficient for collisions ejecting sensor atoms. Under ideal operating conditions, these rate coefficients are immutable physical quantities that can be determined from fundamental *ab initio* theoretical quantum calculations or extracted from measurements. The resulting measurement equation for pressure,

$$p = \frac{\Gamma}{L}kT \tag{1}$$

has two immutable constants, L and k, and two measured quantities Γ and T. Thus, the CAVS is traceable to the SI second and kelvin.

So far, we have implicitly assumed that the vacuum only contains a single atomic or molecular species. This



FIG. 1. Expected lithium-based CAVS lifetime $\tau = 1/\Gamma$ as a function of pressure for XHV, UHV, and high vacuum (HV) containing only H₂ molecules at a temperature of 300 K.

assumption is not unreasonable, as with current technology hydrogen molecules tend to be the dominant background species in XHV and UHV environments. Vacuum chambers, properly prepared for UHV and XHV, outgas predominately hydrogen. Figure 1 shows the predicted lifetime $\tau = 1/\Gamma$ as a function of pressure in the XHV and UHV domain for a lithium-based CAVS assuming that only room-temperature H₂ molecules are present in the vacuum chamber. The timescales range from 100 s in the UHV up to a challenging one day in the XHV.

Depending on the application, atomic and molecular species other than H_2 , such as noble gas atoms, N_2 , H_2O , CO_2 , might and will be introduced for leak detection, surface processing, etc. For the proper operation of CAVS, it will thus be important to understand the partial number densities and thus partial pressure of each of the added species. We expect, however, that only a few species will be simultaneously present. Still, we envision that a CAVS will come with a small database of temperature-dependent loss rate coefficients for many relevant species.

This paper describes two realizations of the CAVS at NIST: a laboratory version, simply called the CAVS, and a portable version, dubbed the pCAVS. The laboratory version is intended as a tool to investigate the operation of the CAVS as well as to obtain the lowest uncertainty for pressures and measure loss-rate coefficients. The pCAVS is designed to have a footprint similar to commercially available gauges, potentially with a lower cost.

In the laboratory version, sensor alkali-metal atoms are pre-cooled into a two-dimensional magneto-optical trap

AIP Publishing (2D MOT). Their residual longitudinal velocity (orthogonal to the plane of the 2D MOT) propels them through a small tube into a separate region where they are further cooled in a three-dimensional magneto-optical trap (3D MOT) to sub-millikelvin temperatures. Cooling lasers are then turned off and sensor atoms are transferred to an Ioffe-Pritchard³⁰⁻³⁴ or a quadrupole^{33,35} magnetic trap. After a delay time, the cooling lasers are again turned on, remaining sensor atoms are gathered into a 3D MOT, and a fluorescence image is used to deduce the loss of sensing atoms from the magnetic trap. By repeating these steps with different delay times, the atom trap lifetime is extracted.

Of course, the proper operation of our CAVSs must be verified. We can do so by setting a known pressure of an atomic or molecular species of interest with the dynamic expansion technique. In practice, this known pressure will be between 10^{-7} Pa and 10^{-6} Pa, where the CAVS experimental timescales are not yet challenging and limits on pumping speeds in the dynamic expansion system have not been reached. With this known pressure and measured Γ by the CAVS an experimental value for K_{loss} for each atomic or molecular species of interest is found. This experimental value can be compared to theoretical calculations of the loss rate coefficient.

In its simplest implementation, a dynamic expansion device has two chambers connected by an orifice and relies on the validity of free molecular flow, where the mean free path of particles in the gas is much larger than the chamber sizes and orifice diameter. The laboratory CAVS is connected to the first chamber. The orifice has a species-dependent conductance C_0 determined from its spatial dimensions and a Monte Carlo simulation of the gas passing through the orifice. Next, a known gas throughput q, which is related to flow \dot{n} with unit mol/s in the SI through $q = \dot{n}RT$, is generated and measured by a flowmeter, is directed into a first chamber, and exits through the orifice into the second chamber. Gas is then rapidly pumped out of the second chamber. This leads to a pressure difference $\Delta p = qRT/C_0$ across the orifice, where $R = kN_A$, N_A , and T are the molar gas constant, Avogadro's constant, and the temperature of the gases in the dynamic expansion standard, respectively. In addition, the ratio of pressures in the two chambers, $r_{\rm p}$, is measured and some algebra shows that the pressure in the first chamber is $p = (r_{\rm p}/[r_{\rm p}-1])qRT/C_0$.

The physics of the pCAVS is the same as that for the CAVS, but there are important technical differences between the two designs. These design differences allow for a much smaller construction and lower cost at the expense of a higher uncertainty of the pressure measurements. First, much of the laser-cooling optical system is replaced by a nano-fabricated grating that allows a single laser beam incident upon the grating to perform Zeeman slowing and cooling and create a tetrahedral-like 3D MOT.³⁶ The pCAVS can be operated in a slow mode, where sensor atoms are transferred from the 3D MOT to a quadupole magnetic trap or a fast mode, where the 3D MOT is used as the sensing trap. The former has the advantage of leading to lower uncertainties, while the latter has the advantage of simpler operation and faster measurement of vacuum pressures.

The remainder of this paper describes our understanding and building of the CAVS and pCAVS. In Section II, we introduce the pertinent atomic and molecular physics required to understand collisions in a CAVS and discuss fundamental limits of a CAVS. We also describe recent published *ab initio* calculations of loss rate coefficients for $Li+H_2$ and Li+He collisions. In Sec. III, we describe how we prepare the smallest pressures possible, the implementation of the dynamic expansion system and flowmeter to set a know gas flow. The CAVS and pCAVS are described in detail in Sections IV and V, respectively, including a discussion of the design of the two- and threedimensional MOTs and magnetic field coils for the final magnetic atom traps. For the pCAVS, this also includes a discussion of the fabrication of the nano-grating. The three sections are mostly self-contained and can be read independently.

II. ATOMIC AND MOLECULAR THEORY FOR THE COLD-ATOM VACUUM SENSOR

In this section, we summarize the collisional physics relevant for the cold-atom vacuum sensor. We introduce the rate equation for loss of sensor atoms, which naturally leads to limits on CAVS operation due to collisions *among* ultra-cold sensor atoms, in Secs. II A and IIB. We restrict the discussions to implementations of CAVSs based on either ultra-cold ⁷Li or ⁸⁷Rb atoms held in magnetic traps. Details regarding the experimental implementation of magnetic atom traps can be found in Sec. IV. Next in this theoretical section, we explain the kinematics of sensor-atom loss from collisions with background atoms and molecules in Sec. IIC and show that nearly all momentum-changing collisions lead to loss. Additional limits on the CAVS, due to glancing or heating collisions that do not impart sufficient momentum to the sensor atom for ejection from the trap, are then described in Sec. IID. The role of the magnetic trap design on glancing collisions is briefly discussed. Formal expressions for scattering amplitudes, glancing collision rates, and thermalized rate coefficients with gases at two temperatures are summarized in Secs. II E and II F. Semiclassical approximations lead to useful analytical expressions for these quantities and are described in Sec. II G. In Sec. II H, we summarize published rate coefficients for Li+H₂ collisions based on the best available interaction potentials between these atoms and numerical evaluations of the collisional rate coefficients. The best values for the rate coefficients significantly differ from those based on semi-classical approximations for this system.

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A. Model for the loss of sensor atoms in magnetic traps

The basic principles of the CAVS have been described

dependent sensor atom number density

$$\frac{\mathrm{d}\rho_c(\mathbf{x},t)}{\mathrm{d}t} = -(\Gamma + \gamma)\,\rho_c(\mathbf{x},t) - K_2\rho_c^2(\mathbf{x},t) - K_3\rho_c^3(\mathbf{x},t)\,.$$
(2)

The term $-\Gamma \rho_c(\mathbf{x}, t)$ on the right hand side of Eq. (2) describes sensor atom loss from collisions with background gas species with rate $\Gamma = \sum_i L_i \rho_i$. Each species *i* in the vacuum chamber adds term $L_i \rho_i$ to Γ , where ρ_i is its number density and L_i is the rate coefficient for loss of a sensor atom. A discussion of the L_i 's is postponed until Sec. II E.

The term $-\gamma \rho_c(\mathbf{x}, t)$ in Eq. (2) indicates small, unwanted sensor atom loss with $\gamma \ll \Gamma$. In a quadrupole trap, the Majorana process,⁴¹ where sensor atoms pass through the zero-field position and change their hyperfine projection state (or colloquially, "flip their spin"), can be such a process. In practice, even for 100 μ K sensor atoms the Majorana process is slow. The depth of quadrupole and Ioffe-Pritchard magnetic traps is often controlled by applying resonant RF radiation, a so-called RF knife⁴². For details on the how the RF fields are generated, see Sec. IV.

The last two terms in Eq. (2) represent approximate descriptions of losses from two- and three-body collisions among sensor atoms with rate coefficients K_2 and K_3 , respectively, thermalized assuming a Maxwell-Boltzmann momentum distribution at temperatures below or around 100 μ K. We will assume $\rho_c(\mathbf{x}, t) = \rho_{c0}$ is a constant, homogeneous sensor-atom number density at the start of pressure measurements for the remainder of this section. A collision between two ultra-cold alkali-metal atoms can change the hyperfine state of the atoms with accompanying increase in relative kinetic energy and loss of both atoms. These cold collisional processes are unavoidable for the $|1, -1\rangle$ and $|2, 2\rangle$ hyperfine states as there exist states with lower energy $E_{\rm hf}$. More subtly, momentumchanging elastic collisions between two sensor atoms can lead to loss of one of them when its kinetic energy becomes larger than the depth of the magnetic trap. This evaporative-loss process contributes to K_2 . Finally, the rate coefficient K_3 describes three-body recombination where three ultra-cold atoms collide to form a di-atomic molecule. Both the molecule and the remaining atom are lost from the trap when their relative kinetic energy is significantly larger than the trap depth.

Equation 2 has several limitations, which concern its dependence on initial sensor-atom number density ρ_{c0} . As sensor atoms are lost by ultra-cold two- and three-body collisions, the cold-atom number density decreases and changes its shape as more atoms are lost where the number density is highest, *i.e.* near the center of the trap where the atomic kinetic energies are smallest. On the other hand, elastic momentum-changing collisions among the cold atoms redistribute the atom cloud to a new thermal density profile. The relevant timescale is the mean free time between collisions $\tau_{\rm elas} = 1/(K_{\rm elas}\rho_{c0})$, where $K_{\rm elas}$ is the total thermalized elastic rate coefficient. See, for example, the analyses in Refs. 43 and 44

in the introduction. Here, we revisit these principles focusing on some theoretical limits on its operation. The atoms of choice are laser-cooled ⁷Li or ⁸⁷Rb alkali-metal atoms with their ²S electronic ground state corresponding to a total electron angular momentum quantum number of 1/2. These isotopes also have non-zero nuclear spins. In fact, both ⁷Li and ⁸⁷Rb have nuclear spin quantum number 3/2. The electron angular momentum and nuclear spin are coupled by the Fermi-contact interaction and the Zeeman interaction when a magnetic field \vec{B} is applied.^{37,38} The corresponding hyperfine eigenenergies $E_{\rm hf}$ of the electronic ground-state of ⁷Li as functions of magnetic field strength B are shown in Fig. 2(a) up to B = 10 mT. The *B*-field-dependent eigenstates $|F, M\rangle$ are labeled by the zero-field quantum numbers F and M of the total atomic angular momentum \vec{F} , the sum of the electronic and nuclear angular momenta. The projection of \vec{F} along the magnetic field with quantum number M is a conserved quantity. Near zero magnetic field strength the slope $dE_{\rm hf}/dB \approx (-1)^F M \mu_{\rm B}/2 \approx$ $(-1)^F M(k \times 340 \ \mu \text{K})/\text{mT}$, where μ_{B} is the Bohr magneton. The equivalent graph for the ⁸⁷Rb atom has the same number of eigenstates, has a qualitatively similar structure, and the same approximate slopes $dE_{\rm hf}/dB$ for small B.

In the CAVS, ultra-cold sensor atoms will be held near the magnetic field zero in a quadrupole trap or near a magnetic field minimum in an Ioffe-Pritchard trap. Magnetic field gradients in quadrupole traps are of the order of 20 mT/cm, while in the Ioffe-Pritchard trap the minimum field strength is on the order of 1 mT with curvature of order 10 mT/cm².

For both quadrupole and Ioffe-Pritchard traps, the preferred atom states to sense pressure are the stretched states with |M| = F. That is, for both ⁷Li and ⁸⁷Rb and our small magnetic field strengths, states $|1, -1\rangle$ and $|2, 2\rangle$ are natural choices. Sensor-atom clouds have temperatures near 100 μ K, spatial dimensions on the order of 1 mm, and a typical mean initial number density of 10^8 cm^{-3} . Finally, remember that in a "clean" UHV environment H₂ is by far the dominant gas.

A model for the number density of cold sensor atoms $\rho_c(t)$, all prepared in a single hyperfine state, as a function of hold time after the preparation of the sample in a magnetic trap should rightly start from the quantum Boltzmann equation for the single-particle phase-space density $F(\vec{x}, \vec{p}, t)$ at time t with position \vec{x} and momentum \vec{p} .^{39,40} Under reasonable assumptions, such as that background species are in thermal equilibrium and have a uniform and time-independent number density, it is sufficient to analyze the differential equation for the spatially-

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FIG. 2. Limits on CAVS operation due to collisions among the ultra-cold sensor atoms. Panel (a) shows the hyperfine energies $E_{\rm hf}$ of the electronic ground state of ⁷Li as functions of magnetic field strength *B*. States are labeled by $|F, M\rangle$ described in the text. States $|1, -1\rangle$ and $|2, 2\rangle$ (blue curves) are most convenient for trapping in a magnetic trap. Panel (b) shows the relationships between various collision rates (bottom *x* axis) or time scales (top *x* axis) and ⁷Li number densities typical for a lithium-based CAVS. The lithium sensor atoms have a temperature of 100 μ K and B = 0.1 mT. The grey band shows rates for the loss of lithium atoms due to collisions with room-temperature H₂ molecules at pressures *p* in the UHV domain between 10^{-9} Pa and 10^{-6} Pa. The magenta lines represent 2-body loss rates for hyperfine-state-changing lithium-lithium collisions. Data for both $|1, -1\rangle$ and $|2, 2\rangle$ are shown. The red line represents sensor atom loss due to three-body recombination to form Li₂ dimers. For ⁷Li only an upper bound for this rate is available. Finally, blue lines represent the mean time between elastic ⁷Li collisions at a temperature of 100 μ K and B = 0.1 mT. The gray band is now only an estimate of timescales due to ⁸⁷Rb+H₂ collisions based on a semiclassical model. The error in this estimate is less than a factor of two.

of cooling and heating of atomic gases in magnetic traps. In the Wigner threshold regime or the zero temperature $limit^{37,45}$,

$$K_{\rm elas} \to \langle v_{\rm rel} \rangle 4\pi a^2$$
 (3)

with thermally-averaged mean relative velocity $\langle v_{\rm rel} \rangle$ and collision-energy-independent scattering length *a*. For ⁷Li the Wigner-threshold limit holds for temperatures up to a few hundred microkelvin, while for ⁸⁷Rb gases this limit is only reached for temperatures below 50 μ K as a *d*-wave shape resonance exists at collision energies of approximately $k \times 300 \ \mu$ K.

Figures 2(b) and (c) show the background loss rate Γ , hyperfine-changing collision loss rate $K_2\rho_{c0}$, and threebody recombination loss rate $K_3\rho_{c0}^2$ from Eq. (2), as well as the thermalization rate $K_{\rm elas}\rho_{c0}$ as functions of typical sensor-atom number density ρ_{c0} for a ⁷Li- and ⁸⁷Rbbased CAVS, respectively. The figure also shows the corresponding timescales $1/\Gamma$, $1/(K_2\rho_{c0})$, $1/(K_3\rho_{c0}^2)$, and $1/(K_{\rm elas}\rho_{c0})$. The samples of sensor atoms have a temperature of 100 μ K. The thermalization time is the only time scale that significantly depends on sensor atom temperature. In fact, decreasing the temperature by a factor of 100 decreases rate $K_{\rm elas}\rho_{c0}$ by a factor of ten. The origin of the values for K_2 , K_3 , and $K_{\rm elas}$ are discussed in Sec. II B. Values for Γ are discussed in Secs. II G and II H.

The background-gas-induced sensor-atom loss rate Γ is independent of sensor-atom number density and gives

the vertical band in Figs. 2(b) and (c). Thus, the time it takes to "sense" pressure at room-temperature UHV pressures lies between 1 s and 1000 s. We want loss from cold hyperfine-changing collisions, and three-body recombination to be small for these time intervals. That is, we require $K_2\rho_{c0}$ and $K_3\rho_{c0}^2$ to be much smaller than Γ , which can be achieved by making the mean sensoratom number density as small as technically realistic. Experimentally, a smaller mean sensor-atom number density also implies a smaller number of atoms N_c and thus requiring tailored atom-counting techniques.

Rates for atom loss from two-body hyperfine-changing collisions are small with the exception of that for the $|2,2\rangle$ hyperfine state. In fact, we do not recommend the use of the $|2,2\rangle$ states to measure pressure in the UHV except when using small mean sensor-atom number densities. Three-body recombination is negligible except for the larger, 10^{12} cm⁻³ number densities and pressures in the XHV where $\Gamma < 10^{-3}$ s⁻¹. Finally, rates $K_{\text{elas}}\rho_{c0}$ for thermalizing collisions are sufficiently large for 100 μ K gases that the momentum distribution of the cold gas will remain close to a thermal equilibrium. Finally, at typical CAVS sensor atom densities of $\rho_{c0} \sim 10^8$ cm⁻³ and temperatures of 100 μ K, the rate of thermalizing collisions is $\Gamma \sim 10^{-2}$ s⁻¹ and is insufficient for maintaining thermal equilibrium.

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B. Inelastic and elastic collisions among the sensor atoms

In this subsection, we present the two-body inelastic and elastic rate coefficients as well as three-body recombination rate coefficients for collisions among sensor atoms used to create Fig. 2. Some data are based on theoretical calculations, others are taken from experiments. We assume that the sensor atoms are in a magnetic field of strength B = 0.1 mT and at a temperature of 100 μ K. Thermally- or Boltzmann-averaged twobody inelastic rate coefficients K_2 are based on numerical coupled-channels calculations using electronic Born-Oppenheimer potentials by Refs. 46 and 47 for 7 Li and ⁸⁷Rb, respectively. For a description of the coupledchannels method as well as a numerical implementation see, for example, Ref. 48. The thermally-averaged inelastic two-body rate coefficients for the $|2,2\rangle + |2,2\rangle$ collision are $K_2 = 3.2 \times 10^{-14} \text{ cm}^3/\text{s}$ and $14 \times 10^{-14} \text{ cm}^3/\text{s}$ for ⁷Li and ⁸⁷Rb, respectively. Those for the $|1, -1\rangle + |1, -1\rangle$ collision are $K_2 = 9.6 \times 10^{-18} \text{ cm}^3/\text{s}$ and 1.6×10^{-14} cm³/s, respectively. In all cases, hyperfine-changing collisions or spin flip collisions are due to the magnetic-dipole magnetic-dipole interaction and, if present, the secondorder spin-orbit interaction.⁴⁹ It is worth noting that in Ref. 50 the researchers measured $K_2 = 2.1(2) \times 10^{-14}$ cm^3/s at B = 100.4 mT and $T = 2 \ \mu\text{K}$ for a gas of $|2,2\rangle$ ⁷Li atoms in agreement with coupled-channels calculations at this field strength and temperature. The number in parenthesis corresponds to a standard deviation uncertainty.

The ⁷Li $|2, 2\rangle$ three-body recombination rate coefficient has not been measured for $B \approx 0.1$ mT. In Ref. 50, however, the researchers measured a ⁷Li $|2, 2\rangle$ recombination rate of $K_3 < 3 \times 10^{-27}$ cm⁶/s in a thermal gas at $T = 2 \ \mu$ K and B = 100.4 mT. We use this upper limit and assume the same upper limit for $|1, -1\rangle$ ⁷Li gases for determining constraints on the lithium-based CAVSs operation. It is worth noting that the resonant *B* dependence of K_3 in a thermal ultra-cold $|1, +1\rangle$ ⁷Li gas near its magnetic Feshbach resonance⁵¹ at B = 73.7 mT has been studied extensively.^{52,53} A three-body recombination rate coefficient of $K_3 = 4.3(1.8) \times 10^{-29}$ cm⁶/s in a $T = 0.8 \ \mu$ K $|1, -1\rangle$ ⁸⁷Rb gas and small *B* fields has been published in Ref. 54. We use this value for determining constraints on the rubidium-based CAVSs operation. We assume the same value for the $|2, 2\rangle$ ⁸⁷Rb state.

The total two-body elastic rate coefficients $K_{\rm elas}$ are also based on coupled-channels calculations. We find that in the limit of zero collision energy, ⁷Li in hyperfine state $|2,2\rangle$ has a scattering length of $a = -28a_0$, where $a_0 \approx 0.0529$ nm is the Bohr radius. For ⁷Li in the $|1,-1\rangle$ state the scattering length is $a = +7.1a_0$ at B = 0.1 mT. At a temperature of 100 μ K and B = 0.1mT, $K_{\rm elas} = 1.8 \times 10^{-11}$ cm³/s and $K_{\rm elas} = 1.5 \times 10^{-12}$ cm³/s for the $|2,2\rangle$ and $|1,-1\rangle$ states, respectively. Consequently, the mean free times between collisions at mean number density $\rho_{c0} = 10^8$ cm⁻³ are $\tau = 550$ s and 6500 s, respectively. Ultra-cold ⁸⁷Rb has a scattering length $a = 100a_0$ for both hyperfine states $|2,2\rangle$ and $|1,-1\rangle$. At a temperature of 100 μ K and B = 0.1 mT, $K_{\rm elas} = 1.4 \times 10^{-10}$ cm³/s and $K_{\rm elas} = 1.2 \times 10^{-10}$ cm³/s for these two ⁸⁷Rb hyperfine states, respectively. Hence, the mean free time between collisions at $\rho_{c0} = 10^8$ cm⁻³ is $\tau = 70$ s and 80 s, respectively.

C. Kinematics of atom-molecule collisions

The kinematics of particle momenta in collisions among room-temperature atoms or molecules and ultracold atoms is key to understanding the loss of sensor atoms in the CAVS.^{37,44,55} For our purposes, it is sufficient to only consider the elastic, momentum-changing collision of a hot, room-temperature particle with mass m_h and initial momentum \vec{p}_h and a cold sensor atom with mass m_c at rest in a potential that only depends on the separation between the center of masses of the particles. After the collision, the momenta of the hot particle and sensor atom are \vec{q}_h and \vec{q}_c , respectively. See Fig. 3(a) for a schematic of such collision. A sensor atom is only lost from its confining trap when its kinetic energy $\epsilon_c \equiv q_c^2/(2m_c)$ is greater than the energy or trap depth W of the confining trap. Cautionary observations about the underlying assumptions are found in Sec. IID.

For the next step in the analysis, we note that the center-of-mass momenta before and after the elastic collision are $\vec{P}_{\rm CM} = \vec{p}_h$ and $\vec{Q}_{\rm CM} = \vec{q}_h + \vec{q}_c$, respectively. Similarly, initial and final relative momenta are

$$\vec{p}_{\rm rel} = \frac{m_c \, \vec{p}_h}{m_h + m_c} \quad \text{and} \quad \vec{q}_{\rm rel} = \frac{m_c \, \vec{q}_h - m_h \, \vec{q}_c}{m_h + m_c} \,, \qquad (4)$$

respectively. We also define velocities $\vec{u}_i = \vec{p}_i/m_i$ and $\vec{v}_i = \vec{q}_i/m_i$ with i = h or c and relative velocities $\vec{u}_{\rm rel} = \vec{p}_{\rm rel}/\mu$ and $\vec{v}_{\rm rel} = \vec{q}_{\rm rel}/\mu$, where reduced mass μ is found from $1/\mu = 1/m_h + 1/m_c$. After some algebra, momentum and energy conservation then imply for the relative kinetic energy

$$E \equiv \frac{p_{\rm rel}^2}{2\mu} = \frac{q_{\rm rel}^2}{2\mu} = \frac{p_h^2}{2m_h} \times \frac{\mu}{m_h} \,. \tag{5}$$

It is proportional to the incoming kinetic energy $p_h^2/(2m_h)$ of a room-temperature particle.

Elastic differential rate coefficients and cross sections for scattering in a potential that only depends on the separation between the particles are most concisely expressed in terms of the relative kinetic energy E and collision angle θ between the final and initial relative momenta, $\vec{q}_{\rm rel}$ and $\vec{p}_{\rm rel}$ or, equivalently, between relative velocities $\vec{u}_{\rm rel}$ and $\vec{v}_{\rm rel}$ (See Fig. 3(b).) With our sensor atom initially at rest, we derive

$$\sin^2(\theta/2) = \frac{1}{4} \frac{m_c}{\mu} \frac{\epsilon_c}{E}.$$
 (6)

In a CAVS, atoms are lost when $\epsilon_c > W$ and, thus, for relative kinetic energy E, Eq. (6) implies that for

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Kinematics of elastic scattering between room-FIG. 3. temperature molecules and ultra-cold atoms. Panel (a) shows the initial momentum \vec{p}_h of a hot H₂ molecule colliding with an ultra-cold lithium (Li) atom, here at rest, as well as momenta \vec{q}_h and \vec{q}_c of H₂ and Li after the collision, respectively. Panel (b) defines the collision angle θ between the final and initial relative velocities, \vec{v}_{rel} and $\vec{u}_{rel} = \vec{u}_h$, respectively. The inset, panel (c), shows Jacobi coordinates R, r, and θ_{iac} for the non-reactive collision between H₂ and Li. Our numerical calculations of (differential) cross sections and rate coefficients have used this coordinate system.

 $\theta > \theta_{\rm c}(E)$ sensor atoms are lost. Here, critical angle $\theta_c(E)$ is defined by

$$\sin^2(\theta_c/2) \equiv \frac{1}{4} \frac{m_c}{\mu} \frac{W}{E} = \frac{1}{4} \frac{m_h + m_c}{\mu} \frac{W}{p_h^2/(2m_h)}.$$
 (7)

The second equality is found with the help of Eq. (5). For $\theta < \theta_{\rm c}(E)$ sensor atoms undergo glancing collisions, where the increase of their kinetic energy is not sufficient for trap loss. Equation (7) implies that for smaller (larger) E, collisions with larger (smaller) collision angles are needed for the loss of a sensor atom.

For intuition regarding typical values for $\theta_{\rm c}(E)$, we note that nominally $p_h^2/(2m_h) \approx kT$ with $T \approx 300$ K and nominal $W/k \approx 100 \ \mu$ K. In addition, mass ratio $(m_h +$ $(m_c)/\mu \geq 4$ and approaches $\max(m_c/m_h, m_h/m_c) \gg 1$ for large mass imbalances, but still we have

$$\sin^2(\theta_{\rm c}/2) \ll 1 \tag{8}$$

for most relative kinetic energies important for a 300 K Maxwell-Boltzmann distribution. In fact, for ultra-cold ⁷Li and ⁸⁷Rb with H₂ background gas, we have $\theta_{\rm c} \approx$ $0.08^{\circ} \times \sqrt{W/(k \times 100 \,\mu\text{K})}$ and $0.2^{\circ} \times \sqrt{W/(k \times 100 \,\mu\text{K})}$, respectively. This angle θ_c is small and promising for CAVS operation but only tells part of the story. As we review in the next few subsections the strong θ dependence of the elastic cross section near $\theta = 0$ also plays a role.

D. Limits from the kinematics on the CAVS

Several cautionary observations about the assumptions in the kinematic model for the operation of the CAVS must be made. First, the role, if any, of inelastic statechanging collisions should be considered. For example,

the potential between an atom and a H₂ molecule does not only depend on pair separation, but also the orientation of the molecule. In a collision, this orientation dependence can lead to changes in the ro-vibrational state of H_2 . A change in the internal state of an atom or molecule is nearly always significantly larger then the depth of the sensor-atom trap. Thus, inelastic collisions lead to loss of sensor atoms. On the other hand, Ref. 56 showed that, in Li and H₂ collisions, rate coefficients for ro-vibrational transitions in H₂ are small compared to the elastic one. Then sensor atom loss is dominated by momentum changes due to elastic collisions. This analysis, however, will need to be redone for each molecular trace element entered into the vacuum chamber.

Second, we have assumed that sensor atoms are initially at rest in the derivation of the kinematics. Sensor atoms, however, do move in the confining trap and strictly speaking this motion must be accounted for in the analysis. We, however, do not believe that this approximation is currently limiting our understanding of the CAVS.

Third, the fast atoms and molecules after an elastic collision can remove more ultra-cold sensor atoms on their way out of the cold cloud by additional collisions. The likelihood of such processes is small and can be estimated from the mean free path between collisions given by length $\ell = 1/(\rho_{c0}\sigma_{add})$, where ρ_{c0} is the sensor-atom number density and cross section σ_{add} is either $\sim L/v_h$ when the background species molecule collides with another ultra-cold sensor atom before it leaves the 1 mm size of the sensor atom cloud or $\sim K_{\rm elas}/v_c'$ when the ejected sensor atom collides with another ultra-cold sensor atom. Here, v'_c is a typical velocity of a sensor atom after its collision with a background species and is larger than the escape velocity $v_e = \sqrt{2W/m}$. We find that ℓ in both cases is orders of magnitude larger than sensor atom cloud size.

Finally, the depth of magnetic traps can and will depend on the orientation along which a sensor atom leaves, *i.e.* the direction of $\vec{q_c}$. However, chaotic motion in these anisotropic and anharmonic traps will make the cold atom find a route out of the trap after a relatively short time before it can, for example, collide with other stillcold sensor atoms. We assume that depth W corresponds to the shallowest trap depth.

E. Loss rate coefficients for isotropic interactions

Collision theory^{37,45,55} describes how scattering observables can be computed from the solutions of (coupled) Schrödinger equations for the motion of the center of masses of atoms and molecules in the potentials generated by their electrons. We define these observables for collisions in isotropic, central potentials, that only depend on the separation R between center of masses of the colliding particles.

For an isotropic interaction potential, the Schrödinger

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equation can be solved for each relative orbital angular momentum or partial wave $\ell = 0, 1, 2, \cdots$ and relative collision energy E. The solution or wavefunction of this equation approaches $\sin(kR - \ell\pi/2 + \eta_{\ell}(E))$ for large R, where k is the relative wavenumber, defined by $E = \hbar^2 k^2 / (2\mu)$, and $\eta_{\ell}(E)$ is the real-valued scattering phase shift that encapsulates the effects of the interaction potential. A scattering amplitude is then constructed with

$$f(E,\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell+1) \left(e^{2i\eta_{\ell}(E)} - 1 \right) P_{\ell}(\cos\theta) \,, \quad (9)$$

where $P_{\ell}(x)$ is the Legendre polynomial of degree ℓ . The total elastic rate coefficient is $v_{\rm rel}\sigma(E)$ with $v_{\rm rel} = \hbar k/\mu$ and total elastic cross section

$$\sigma(E) = 2\pi \int_0^\pi \sin\theta d\theta \, |f(E,\theta)|^2 = \frac{4\pi}{k} \operatorname{Im} f(E,\theta=0) \,,$$
(10)

where second equality is obtained the help of the optical theorem.

A thermally-averaged loss rate coefficient L appearing in Eq. (2) is given by

$$L = \langle v_{\rm rel} \sigma(E) \rangle_{\rm eff} - \langle v_{\rm rel} \sigma_{\rm gl}(E) \rangle_{\rm eff} \,, \tag{11}$$

where the glancing-collision cross section

$$\sigma_{\rm gl}(E) = 2\pi \int_0^{\theta_c(E)} \sin\theta d\theta \, |f(E,\theta)|^2 \qquad (12)$$

describes the cross section for collisions that do not impart sufficient momentum for the sensor atom to leave the trap. It is a function of E only. Moreover, in the limit that the sensor atom temperature and trap depth go to zero $L \to \langle v_{\rm rel} \sigma(E) \rangle_{\rm eff}$, the thermally averaged total elastic rate coefficient.

The brackets $\langle \cdots \rangle_{\text{eff}}$ describe a thermal average over a Boltzmann distribution for a sensor atom gas close to zero temperature and a Boltzmann distribution for a background gas species at temperature T_h close to room temperature. Thermally averaging an observable $\mathcal{O}(E)$ only depends on the relative collision energy E

$$\langle \mathcal{O}(E) \rangle_{\text{eff}} = \frac{1}{Z(T_{\text{eff}})} \int_0^\infty \sqrt{E} \mathrm{d}E \,\mathcal{O}(E) e^{-E/kT_{\text{eff}}}, \quad (13)$$

where the effective temperature is given by

$$T_{\rm eff} = \frac{m_c}{m_c + m_h} T_h \tag{14}$$

and $Z(T) = \int_0^\infty \sqrt{E} dE e^{-E/kT}$. For later use, we realize

$$\langle E^s \rangle_{\text{eff}} = \frac{\Gamma(3/2+s)}{\Gamma(3/2)} (kT_{\text{eff}})^s \tag{15}$$

when s > -3/2 and $\Gamma(x)$ is the Gamma function with $\Gamma(x+1) = x\Gamma(x).$

Finally, it is convenient to define the fraction or probability of glancing collisions

$$P_{\rm gc} = \frac{\langle v_{\rm rel}\sigma_{\rm gl}(E)\rangle_{\rm eff}}{\langle v_{\rm rel}\sigma(E)\rangle_{\rm eff}} \ll 1.$$
 (16)

F. Small angle scattering for isotropic interactions

In Sec. II C on the kinetics of the CAVS we defined an energy-dependent critical angle $\theta_c(E)$, such that when the scattering angle θ between final and initial relative momenta is less than $\theta_c(E)$ the sensor atoms cannot leave the magnetic trap after the collision. As $\theta_{\rm c}(E) \ll 1$, we can derive small angle expansions of Eqs. (9) and (12)using

$$P_{\ell}(\cos\theta) = 1 - (\ell+1)\ell\sin^2(\theta/2) + O\left(\ell^4\sin^4(\theta/2)\right)$$
(17)

for the Legendre polynomial. Here, the big-O notation O(x) describes the limiting behavior of the next term in the expansion. Consequently, at a fixed relative collision energy E the scattering amplitude for an isotropic interaction potential is

$$f(E,\theta) = g_0(E) + g_1(E)\sin^2(\theta/2) + \cdots$$
 (18)

with complex-valued

$$g_0(E) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell+1)(e^{2i\eta_\ell(E)} - 1)$$
(19)

and

$$g_1(E) = -\frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell+1)(\ell+1)\ell \left(e^{2i\eta_\ell(E)} - 1\right). \quad (20)$$

It is important to realize that the expansion in Eq. (17)is only valid when both θ and partial wave ℓ are small, but that to evaluate $f(E, \theta)$ we must sum over all $\ell > 0$. Thus convergence of the expansion on the right hand side of Eq. (18) is not guaranteed. In fact, for our neutral systems with their long-range attractive van-der-Waals interaction the next term for $f(E,\theta)$ represented by an ellipsis in Eq. (18) does not converge. We suspect that this term is not simply proportional to $\sin^4(\theta/2)$. The coefficients $g_0(E)$ and $g_1(E)$ are finite and can be used to describe small angle scattering.

We then derive that the small angle expression for the cross section for glancing collisions is

$$\sigma_{\rm gl}(E) = 4\pi |g_0(E)|^2 \sin^2(\theta_c/2)$$
(21)
+ $4\pi \operatorname{Re}[g_0^*(E)g_1(E)] \sin^4(\theta_c/2) + \cdots$

with $\sin^2(\theta_c/2) \propto W/E$ defined in Eq. (7). Finally, for the thermally averaged loss rate coefficient from the CAVS we have

$$L = \langle v_{\rm rel}\sigma(E)\rangle_{\rm eff} - 4\pi \langle v_{\rm rel}|g_0(E)|^2\rangle_{\rm eff}\sin^2(\theta_c/2) - 4\pi \langle v_{\rm rel}{\rm Re}[g_0^*(E)g_1(E)]\rangle_{\rm eff}\sin^4(\theta_c/2) + \cdots (22)$$

G. Semiclassical approximations for isotropic interactions

For large collision energies and isotropic interaction potentials, a semiclassical approximation for small angle scattering θ can be used.⁵⁵ Developed in the 1960s,

$$E_6 = \frac{\hbar^2}{2\mu x_6^2}$$
 and $x_6 = \sqrt[4]{\frac{2\mu C_6}{\hbar^2}}$. (23)

We find $E_6/k = 80.5$ mK for ⁷Li+H₂, based on $C_6 = 82.75E_{\rm h}a_0^{6,56}$ and 44.8 mK ⁸⁷Rb+H₂, based on $C_6 = 137E_{\rm h}a_0^{6,44}$ Here, $E_{\rm h}$ is the Hartree energy. For collision partners with a larger reduced mass, E_6 can easily be an order of magnitude smaller.

For relative collision energies $E \gg E_6$, the partialwave-dependent phase shift for attractive van-der-Waals potentials approaches

$$\eta_{\ell}(E) \to \eta_0 \frac{(kx_6)^4}{\ell^5} = \eta_0 \frac{(E/E_6)^2}{\ell^5}$$
 (24)

with $\eta_0 = 3\pi/32$. Gao^{57,58} gives a useful modern derivation of this limit. A semi-classical approximation for the scattering amplitude of Eq. (9) and cross sections is then found by using the limiting form for $\eta_{\ell}(E)$ for all E and ℓ , replacing the sum over ℓ by an integral over ℓ , and changing to integration variable $2\eta_{\ell}(E)$. The integral can either be solved analytically or approximated with the stationary phase method.

For example, the coefficients $g_0(E)$ and $g_1(E)$ in Eqs. (19) and (20) can be found analytically in the semiclassical approximation and are given by

$$g_0(E) = e^{3\pi i/10} \frac{\Gamma(3/5)(2\eta_0)^{2/5}}{2} \left[\frac{E}{E_6}\right]^{3/10} x_6 \qquad (25)$$

and

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$$g_1(E) = e^{11\pi i/10} \frac{\Gamma(1/5)(2\eta_0)^{4/5}}{4} \left[\frac{E}{E_6}\right]^{11/10} x_6.$$
 (26)

Expressions for the thermally averaged glancingcollision rate coefficient $v_{\rm rel}\sigma_{\rm gl}(E)$ and total elastic rate coefficient $v_{\rm rel}\sigma(E)$ can then be easily derived with the help of Eq. (15). For example, the total elastic rate coefficient is

$$\langle v_{\rm rel}\sigma(E)\rangle_{\rm eff} = b_{\rm tot} \left[\frac{kT_{\rm eff}}{E_6}\right]^{3/10} \frac{\hbar}{\mu} x_6 , \qquad (27)$$

with dimensionless coefficient

$$b_{\rm tot} = 4\sqrt{\pi}\Gamma(3/5)\Gamma(9/5)(2\eta_0)^{2/5}\sin\frac{3\pi}{10} \approx 6.43773\,,$$

and is a slowly increasing function of effective temperature, while the glancing-collision rate coefficient is

$$\langle v_{\rm rel}\sigma_{\rm gl}(E)\rangle_{\rm eff} = \left\{ d_1 \left[\frac{kT_{\rm eff}}{E_6}\right]^{1/10} \frac{m_c}{\mu} \frac{W}{E_6} \qquad (28) \\ - d_2 \left[\frac{kT_{\rm eff}}{E_6}\right]^{-1/10} \left(\frac{m_c}{\mu} \frac{W}{E_6}\right)^2 \right\} \frac{\hbar}{\mu} x_6$$

with

$$d_1 = \frac{\sqrt{\pi}}{2} \Gamma^2(3/5) \Gamma(8/5) (2\eta_0)^{4/5} \approx 1.14992$$

and

$$d_2 = \frac{\sqrt{\pi}}{16} \Gamma(3/5) \Gamma(1/5) \Gamma(7/5) (2\eta_0)^{6/5} \cos \frac{\pi}{5} \approx 0.288065 \,.$$

and has an even weaker temperature dependence. The glancing-collision rate coefficient mainly has a linear dependence on the trap depth W. (Remember from the previous subsection that we suspect that the next term is not proportional to W^3 .)

The fraction of glancing collisions is

$$P_{\rm gc} = \frac{d_1}{b_{\rm tot}} \left[\frac{kT_{\rm eff}}{E_6} \right]^{-1/5} \frac{m_c}{\mu} \frac{W}{E_6}$$

$$- \frac{d_2}{b_{\rm tot}} \left[\frac{kT_{\rm eff}}{E_6} \right]^{-2/5} \left(\frac{m_c}{\mu} \frac{W}{E_6} \right)^2$$
(29)

and is also a simple polynomial in the trap depth W. For the proper operation of the CAVS, $P_{\rm gl}$ must be much smaller than one for vacuum temperatures around 300 K. $P_{\rm gl}$ has a weak dependence on temperature with $[E_6/kT_{\rm eff}]^{1/5} \approx 0.1$. More important is that $W/E_6 \sim$ 10^{-3} for ⁷Li+H₂ and ⁸⁷Rb+H₂ with trap depth W/k =100 μ K. This implies a fraction on the order of 10^{-4} and virtually all collisions with H₂ lead sensor atom loss. Of course, W/E_6 will be significantly larger for heavier reduced-mass systems leading to the need for shallower magnetic traps.

The semi-classical approximations are accurate as long as $|\eta_{\ell}(E)| \gg \pi$ for small ℓ where the limiting form in Eq. (24) is not valid. The validity of the semi-classical approximations is not guaranteed, but nevertheless its predictions for cross sections and rate coefficients are typically accurate to better than 20% and thus are useful to understand the dependencies on temperature and trap depth. In Section II H, we will compare the estimates from the semi-classical theory with exact numerical results for the Li+H₂ collision.

H. Computations of elastic rate coefficients for $\text{Li}+\text{H}_2$ collisions

In the astrophysical community, the reactive LiH + H collision to break up LiH to form hydrogen molecules is

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of ongoing interest.⁵⁹ Both H_2 and LiH are likely the first molecules to have formed in the cooling and expanding universe. The process is exothermic by about 2.26 eV or $k \times 26200$ K. For the CAVS, we are interested in the "inverse" non-reactive collision of Li with H₂ at of order $k \times 300$ K collision energies.

The first quantitative estimate, including an uncertainty budget, of the room-temperature total elastic rate coefficient for ⁷Li+H₂ collisions was published in Ref. 56 and an erratum in $2022.^{60}$ Here, the molecule is in one of the lowest ro-vibrational levels of its ground-electronic $X^1\Sigma_q^+$ state. The authors began their analysis by computing the three-dimensional ²A ground-electronic potential energy surface $V(R, r, \theta_{iac})$ for H-H separations r near the H_2 equilibrium separation, where r is part of the Jacobi coordinates R, r, and θ_{jac} defined in Fig. 3(c). For room-temperature ${}^{7}Li+H_{2}$ collisions, this region in coordinate space is sufficient not only as the activation energy to the $^{7}LiH + H$ arrangement is large, but also as the energy spacing between the lowest vibrational states of H₂ is significantly larger than our typical collision energy. In this region of coordinate space, the potential energy surface is almost isotropic, that is, has a weak angle θ_{iac} dependence, and has a depth of only $k \times 10.6(5)$ K at T-shaped geometries with $r = 1.4 a_0$, close to the H₂ equilibrium separation, This value is small compared to the kinetic energies of H_2 and the number in parenthesis is its one-standard deviation uncertainty.

The authors then performed coupled-channels calculations, that is found numerical solutions of coupled sets of radial Schrödinger equations, in the channel basis constructed from ortho- and para-rovibrational states of the $X^1\Sigma_q^+$ state of the homonuclear H₂ and spherical harmonic functions $Y_{\ell m}(\hat{R})$ describing the rotation of H₂ and ⁷Li around each other. Here, ℓ is the partial wave and \hat{R} is the orientation of the axis connecting the center of masses of H_2 and ⁷Li. The electron and nuclear spins of H_2 and ⁷Li were treated as bystanders and not allowed to change direction during the collision.

The prediction for the total rate coefficient for $^{7}Li+H_{2}$ collisions is

$$\langle v_{\rm rel}\sigma(E)\rangle_{\rm eff} = 3.18(6) \times 10^{-9} \,{\rm cm}^3/{\rm s}$$
 (30)
+1.21(8) × 10⁻¹² cm³/(s K) × (T - 300 K)

based on Refs. 56 and 60, where T is the temperature of the H_2 molecules near 300 K and the numbers in parenthesis are the one-standard deviation uncertainties. In fact, only rovibrational states v = 0 and j = 0 through 4 need to be included. Moreover, inelastic rate coefficients for *j*-changing collisions are orders of magnitude smaller than the total elastic rate coefficient. Equation (30) has been used to create Figs. 1 and 2(b).

Finally, the results of Eq. (30) can be compared with the semiclassical rate coefficient given in Eq. (27). At T = 300 K and $C_6 = 82.75 E_h a_0^6$, we find that the semiclassical rate coefficient underestimates the corresponding quantum prediction by 20%. This 20% difference

is larger than the 2% fractional uncertainty in Eq. (30), but does suggest that semiclassical rate coefficients can be used as a good initial estimate of sensor atom loss rates.

III. GENERATING AND CHARACTERIZING AN **EXTREME-HIGH VACUUM**

A. Vacuum preparation

In order to produce XHV and UHV vacuum levels, a variety of techniques must be combined. In this section we describe the primary mechanism limiting the vacuum level, namely outgassing. (Another possible limitationleaks-can be found and fixed via standard leak checking.) We then turn our attention to mitigation measures including medium- and high-temperature baking to drive hydrogen out of the stainless steel components before assembly and low-temperature baking to remove water from the assembled system. Moreover, we will describe our selection of materials and pumps as well as the strategy for pumping.

1. Gas load limitations on vacuum

The lowest pressure that can be achieved in a vacuum system results from a balance between the gas load into the system, *i.e.* outgassing and leaks, and the rate with which gas is removed. The ability to remove gas is quantified by pump speed S with unit L/s in the SI. Here, S takes into account the pump speed of the pumps but also conductance restrictions between the vacuum system and the pumps. The ultimate pressure is then determined by the total gas throughput into the vacuum system, measured in SI units PaL/s.

There are limits on increasing the pumping speed in the various parts of a vacuum system. For example, our dynamic expansion system has two chambers connected by a small orifice, where only the chamber with the lowest pressure is connected to pumps. Thus the pressure in the other, upstream chamber, to which the CAVS is attached, is determined by conductance of orifice as well as the pumps. Gas pumping is kept to a minimum in this upstream chamber to minimize pressure gradients that could cause inaccuracies in the CAVS pressure reading. Given these design restrictions, we focused on reducing the outgassing rate of our vacuum components.

The majority of our chambers and vacuum components are constructed out of 304L or 316L stainless steel. After the initial evacuation of a vacuum chamber, starting from air at atmospheric pressure, the most abundant outgassing product into the chamber is water desorbing from the steel surfaces. As the desorbed water gas is removed by the vacuum pumps, the specific outgassing rate Q (per unit area) from surfaces decreases, typically approaches a power law in time from the time the pumps are turned

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After water desorption has become negligible by the 100 °C to 150 °C bake, the predominant outgassing species is H_2 . This is due to atomic hydrogen dissolved within the metallic chamber walls. Hydrogen diffuses through the bulk of the metal and combines on the surface to release H_2 gas into the chambers. For untreated stainless steel, the hydrogen specific outgassing rate or flux is on the order of 10^{-9} Pa L s⁻¹ cm⁻² at room temperature.⁶³ However, for the present application, outgassing rates per unit area below 10^{-10} Pa L s⁻¹ cm⁻² are desired to reach XHV. To achieve such low outgassing levels, we bake our stainless steel parts at much higher temperatures than 150 $^{\circ}$ C before we even assemble the vacuum system. Other materials with lower H₂ outgassing flux, such as aluminum or titanium, can also be chosen. Our choice for baking and materials will be discussed in the next subsections.

2. Materials and heat treatments to reduce H₂ outgassing

It is standard practice to construct vacuum systems out of stainless steel because it is resilient against deformation, can withstand mechanical shock, resists oxidation, and can be made non-magnetic. However, as discussed in previous subsections hydrogen is dissolved in bulk stainless steel and leads to a gas load into the vacuum system. The primary contribution to the gas load on a well-constructed vacuum system, typically at a pressures below 10^{-7} Pa for a standard size vacuum chamber, is from H₂ gas desorbing from stainless steel. This disadvantage led us to consider other materials, and to conduct studies of various heat treatments to suppress outgassing.

Some components in our system are made of glass, i.e. windows and the glass cell of the main CAVS apparatus (see Sec. IV), to allow optical access to control and laser cool the sensor atoms. In principle, glass is an excellent material for vacuum, but its brittleness makes it impractical for large systems. Moreover, glass is permeable by light atoms and molecules (H_2 , He). Porous materials like ceramics and alumina have their uses inside vacuum systems, but are not suitable for chamber construction.

Reasonable candidate materials for chamber construction are restricted to machinable metals. In order to compare outgassing from these materials, we constructed geometrically identical chambers out of Al, Ti, and three types of stainless steel: 304L; 316L; and 316LN, (an electroslag remelt). We measured outgassing before and af-

ter heat-treatment. As described in Ref. 62, the chambers are 20 cm long cylinders with an inner diameter of 20 cm. The wall thickness is 3 mm and all interior surfaces have a standard machine finish of better than Ra 1.6 μ m, characterizing the mean of absolute values of surface heights relative to the mean height averaged over the surface. The cylinders are open on one end, terminated in a CF-type knife edge flange. The flange is sealed to a 13 mm thick DN200 flange using a copper gasket for all but the aluminum chamber, for which a gasket made of 1100-H14 series aluminum is used. The thickness of the DN200 flange is reduced from that of a standard DN200 flange to facilitate better degassing of the chambers. Each chamber together with a spinning rotor gauge (SRG) is assembled onto a pumping station via an orifice and shrouded in a custom-made temperature-controlled baking shell.

After the removal of all water from the interior surfaces of the cylinders with a 100 °C to 150 °C low-temperature bake over several days and a return to ambient laboratory temperatures, we measure hydrogen outgassing of the chamber by isolating it from the pump by closing a valve and monitoring the pressure increase for a few hours or days depending on the rate of rise. The rise rate is linear in time and its slope dp/dt is used to calculate the specific outgassing rate (per unit surface area) or outgassing flux of the chamber material

$$Q_{\rm H_2} = \frac{V}{A} \frac{\mathrm{d}p}{\mathrm{d}t} - \frac{q_0}{A} \,, \tag{31}$$

where V and A are the known volume and surface area of the chamber, respectively, and q_0 is the separately measured background outgassing rate of the pumping apparatus capped off without a chamber installed. Table I shows the results of our measurements of $Q_{\rm H_2}$ for various metals with and without a heat treatment consisting of baking at 950 °C for a minimum of 24 h in an vacuum oven with a pressure $< 1 \times 10^{-2}$ Pa. Titanium has the smallest $Q_{\rm H_2}$, while stainless steel that has not undergone heat treatments has a $Q_{\rm H_2}$ that is more than one hundred times worse. Heat treating stainless steel, however, leads to $Q_{\rm H_2}$ that are comparable to that for titanium and we conclude that heat-treated stainless steel is a good choice for our applications. Moreover, stainless steel is readily machinable and weldable, and it is the most common material choice for stock vacuum components.

For large components with thick flanges, steel acts like a nearly infinite H_2 reservoir. There exist two approaches to mitigate this gas source, (1) coating the interior chamber surface to trap hydrogen in the bulk and (2) driving the hydrogen out of the stainless steel reservoir by medium or high temperature bakes. Although coating techniques have shown success in reducing outgassing rates⁶⁴, this method seemed impractical for the large number of chambers and components required for the CAVS and dynamic expansion system, thus most of our effort has been toward the second technique, although we did study controlled air-bakes which deposit an oxide

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	Activ	vation		Relative
Chamber	Energ	gy, $E_{\rm D}$	$Q_{\rm H_2}$	Improvement
Material	(eV)	(K)	$({\rm PaLs^{-1}cm^{-2}})$	Factor
Ti			2.5×10^{-12}	377
Al	0.37	4250	5.5×10^{-12}	172
316L-XHV	0.68	8080	5.1×10^{-12}	184
316LN-XHV	0.53	6890	9.9×10^{-12}	95
316L	0.66	7580	6.5×10^{-10}	1.5
316LN	0.64	7450	$7.0 imes 10^{-10}$	1.3
304L	0.59	6880	9.4×10^{-10}	1.0

TABLE I. Activation energies $E_{\rm D}$ for atomic hydrogen and specific outgassing rates $Q_{\rm H_2}$ of molecular hydrogen at a temperature of 298.15 K for vacuum chambers made out of titanium (Ti), aluminum (Al), and various stainless steel qualities labeled by 316L, 316LN, and 304L. Stainless steel with '-XHV' suffix is steel that has undergone a heat treatment. The relative uncertainty $u(Q_{\rm H_2})/Q_{\rm H_2} = 0.24$ for the 316L, 316LN, and 304L chambers, and 0.72 for all others. The relative improvement factor $Q_{\rm H_2}(304 {\rm L})/Q_{\rm H_2}(M)$ for a chamber made of material M is given in the last column. Reproduced from J. A. Fedchak, J. K. Scherschligt, S. Avdiaj, D. S. Barker, S. P. Eckel, B. Bowers, S. O'Connell, and P. Henderson, J. Vac. Sci. Technol. B 39, 24201 (2021), public domain.

layer onto the chamber surfaces. See Ref. 63 for details.

Medium and high temperature bakes diffuse hydrogen out of stainless steel. The diffusion coefficient of H in stainless steel is proportional to $\exp(-E_{\rm D}/kT)$, where $E_{\rm D}/k \approx 7000$ K is a typical activation energy for diffusion.^{62,65} The activation energy for several different materials are shown in Tab. I. Even modest bakes at 450 °C increase the rate at which hydrogen diffuses to the surface, where it can then recombine to form H_2 and desorb from the surface, by more than a factor 10^6 compared to that at room temperature. Hence, the H₂ desorbtion rate is greatly reduced by heat treatments. A useful table for estimating baking times can be found in Ref. 66.

We baked most of our disassembled components of the CAVS and dynamic expansion system under vacuum and at a temperature between 400 $^{\circ}C$ and 450 $^{\circ}C$, a medium temperature bake. In fact, we constructed our own in-house vacuum furnace to perform these mediumtemperature bakes.⁶⁶ We monitored the pressure during a bake and, thus, the outgassing rate in real time. This enabled us minimize the duration of bakes.

In principle, a high-temperature treatment under vacuum with temperatures greater than 950 $^\circ\mathrm{C}$, often referred to as a vacuum-fire treatment, could have been used. Each bake would require much less time for a similar reduction in the hydrogen outgassing rate than a medium heat-treatment. The disadvantage of a vacuumfire treatment is its cost. An oven capable of producing temperatures exceeding 950 °C under vacuum was not within our budget. Nevertheless, a few components in our system were subjected to vacuum fire by utilizing external vendors with this capability.

It is worth noting that medium-temperature air bakes,

i.e. bakes not performed under vacuum, to reduce hydrogen $outgassing^{67-69}$ can be used. In fact, this technique is used on vacuum components of LIGO.⁷⁰. Our own investigations into air bakes also demonstrated a lowering of hydrogen outgassing but not as low as heat treatments under vacuum for similar chambers at the same temperature.⁶³ Materials evaporating into the air from heaters, insulating materials, etc. can contaminate the surfaces of vacuum components, and it can be difficult to ensure good air flow for small chambers and other small vacuum components.

After the medium- or high-heat treatments, the vacuum components must be assembled into a finished device. Typically, this assembly is done in air containing water vapor, which readily adsorbs on the surface of exposed chamber components. Therefore low-temperature bakes at temperatures between 100 $^{\circ}\mathrm{C}$ and 150 $^{\circ}\mathrm{C}$ must be performed to remove this water. Viewports and other components limit this fully-assembled water bake to temperatures less than 200 °C. After a few days, the pressure in the system stabilizes, at which time the bake is stopped. The pressure will again drop as the system cools to ambient temperature.

B. Dynamic expansion system

Currently, the primary standard at NIST and other National Metrology Institutes to set a known UHV pressure consists of an apparatus that generates a known flow of gas injected into a dynamic expansion system. We use this well-understood technique to verify calculations of loss rate coefficients of sensor atoms described in Sec. II as well as to enable measurement of loss rate coefficients due to gases for which calculations are not available. Moreover, this apparatus provides a helpful diagnostic tool for the CAVS operation. This subsection describes the dynamic expansion system. The flow splitter and flowmeter that are used to create a known flow or gas throughput are discussed in the following subsections.

The principle of dynamic expansion, schematically shown in Fig. 4, is based on gas flow in the free molecular flow regime from a chamber with gas pressure p_1 through an orifice with calculable conductance C_0 to a second chamber with gas pressure p_2 . The CAVS is connected to the first chamber. The flow leads to a pressure difference across the orifice equal to

$$\Delta p = p_1 - p_2 = \frac{\dot{n}RT}{C_0} = \frac{q}{C_0}$$
(32)

for gas flow \dot{n} with unit mol/s or gas throughput q = $\dot{n}RT$. In the limit that $C_0 \ll S$, $p_1 \gg p_2$, and we see that $p_1 \approx q/C_0$. Thus, this first chamber can be used to calibrate vacuum gauges, or potentially validate the CAVS. We note that throughput q may not be conserved as gas flows through multiple chambers, particularly when the chamber temperatures are different, but \dot{n} is.

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This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0120500 The conductance C_0 needs to be calculated accurately for this technique to work. In the molecular flow regime,

$$C_0 = \mathcal{W}A_0 \sqrt{\frac{kT}{2\pi m_h}},\qquad(33)$$

where A_0 is the area of the orifice, m_h is the mass of the hot background atom or molecule, and dimensionless \mathcal{W} is the species-independent transmission probability. Sufficiently accurate approximations for \mathcal{W} are known analytically for circular tubes of diameter D and length L.^{71–75} To wit,

$$\mathcal{W} = 1 + \mathcal{R}^2 - \mathcal{R}\sqrt{\mathcal{R}^2 + 1} - \frac{2}{9} \frac{\left(\mathcal{R}^3 - 2 + (2 - \mathcal{R}^2)\sqrt{\mathcal{R}^2 + 1}\right)^2}{\mathcal{R}\sqrt{\mathcal{R}^2 + 1} - \ln\left(\mathcal{R} + \sqrt{\mathcal{R}^2 + 1}\right)},$$
(34)

where $\mathcal{R} = L/D$. Our orifice is a short tube with D = 22.184(8) mm and L = 5.0462(3) mm and we calculate $\mathcal{W} = 0.81570(5)$.

To compute C_0 , we must also know the temperature of the gas in the dynamic expansion chambers. We measure the temperature of the walls of the chamber, assumed to be in thermal equilibrium with the gas, using four platinum resistance thermometers. Their standarddeviation spread is typically 0.4 K. Using a typical laboratory temperature of 295.0(4) K, we compute that $C_0 = 138.7(1)$ L/s for H₂ and $C_0 = 37.22(4)$ L/s for N₂. Consequently, our evaluation of C_0 is limited by our control of the temperature. Because our geometry is more complicated than the simple tube discussed by Ref. 74, we plan to verify the value of C_0 using Monte Carlo simulations.

In general, the limit of $C_0 \ll S$ is not achievable to our desired accuracy. Thus, we need to be more careful about our analysis. The second chamber of the dynamic expansion system is connected to a large turbomolecular pump and two UHV-rated getter pumps. Even with these pumps, true zero pressure is impossible to create. Instead we rewrite Eq. (32) in terms of the pressure ratio $r_{\rm p} = p_1/p_2$ and p_1 . If we measure $r_{\rm p}$ then

$$p_1 = \frac{r_{\rm p}}{r_{\rm p} - 1} \frac{q}{C_0} \,. \tag{35}$$

even when p_2 is nonzero. Typically, $r_p \gg 1$ so that to a good approximation the contribution to the fractional uncertainty in the pressure of the first chamber, $u(p_1)/p_1$, from the uncertainty of r_p is suppressed and given by $u(r_p)/r_p^2$.

To measure the pressure ratio r_p , we designed our dynamic expansion system with a bypass between the two chambers as shown in Fig. 4 constructed out of DN-40 (40 mm bore) vacuum hardware. The two valves in the bypass are pneumatically actuated all-metal bakeable high-throughput valves (VAT all-metal angle valve, series 57.1) with a spinning rotor gauge (SRG) mounted between them. Spinning rotor gauges are ideally suited schematic e.png schematic e.png



FIG. 4. Schematic of a dynamic expansion system. A known gas input with throughput q (blue arrows) flows into a first chamber. This gas then flows into a second chamber via an orifice with known conductance C_0 and, finally, is pumped away with pump speed S. The pressures in the two chambers are p_1 and p_2 , respectively. The CAVS is connected to the first chamber. Spinning rotor gauges SRG1 and SRG2 and valves V1 and V2 form a bypass with which the ratio of the pressures in the two chambers is measured.

to ratiometric comparisons because they have a linear response with pressure over a wide pressure range and are bakeable.

A single $r_{\rm p}$ measurement consists of first injecting a throughput q into the dynamic expansion system with valves V1 and V2 closed. We then collect the responses of gauge SRG2 by sequentially opening only one of the two valves following pattern V1, V2, V2, and V1. This sequence of measurements determines the pressure in chambers 1, 2, 2, and 1, respectively. Combining the four measurement readings gives $r_{\rm p}$, canceling any linear drift in the gauge indication (typically caused by temperature drifts) and eliminating the need for calibration of gauge SRG2. Six sequences of four measurements are needed to get good statistics.

To be sufficiently above the noise floor of the spinning rotor gauge and ensure a measurement of $r_{\rm p}$ with $u(r_{\rm p})/r_p^2 < 0.01$, we need a flow or throughput that is sufficient to maintain a pressure of ~ 10 mPa in the first chamber, but not larger than 100 mPa as this may exceed the range in which a SRG has a linear response. For CAVS validation, however, $p_1 < 10^{-6}$ Pa is required. Here, we can rely on the fact that $r_{\rm p}$ is independent of throughput q in the molecular flow regime for $p_1 < 0.1$ Pa.

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Finally, it is important to understand the dependence of $r_{\rm p}$ on gas species. For a dynamic expansion system, theoretical analysis shows that

$$r_{\rm p} = \frac{S}{C_0} + 1\,, \tag{36}$$

a simple function of the pumping speed S and the orifice conductance C_0 . We use a combination of a 1500 L/s turbo molecular pump and two 1400 L/s non-evaporable getter pumps for H₂. Thus, $S \approx 4300$ L/s. While the turbo molecular pump is nearly species independent, non-evaporable getter pumps rely on chemical reactions and are therefore highly species dependent. Consequently, the gas-species dependence of $r_{\rm p}$ is more complicated than the $\sqrt{m_h}$ dependence from C_0 and the ratio needs to be measured for each gas species. Finally, as getter pumps become saturated, they are less effective, requiring us to re-measure $r_{\rm p}$ regularly. For H₂, we expect $r_{\rm p} \approx 32$.

C. Optional flow splitter

An optional flow splitter is connected to the dynamic expansion system, as shown in Fig. 5, to further reduce throughput $q_{\rm FM}$ and thus achieve lower pressures in the first chamber of the dynamic expansion system, p_1 . When the gate value shown in Fig. 5 is open, the splitter injects roughly only 1/100 of the flow into the dynamic expansion system; the remainder is diverted into a separate chamber with connecting pumps with pump speed $S_{\rm sp}$. This is accomplished with a spherical chamber and orifices with conductances C_{DE} and C_{DC} . When the gate value is closed, $q = q_{\rm FM}$. For all of the data contained in this paper, the gate valve remains closed and the flow splitter is unused.

The ratio $\alpha = q/q_{\rm FM}$ can be measured using spinning rotor gauge SRG1 with either V1 or V2 closed. Here, $q_{\rm FM}$ is the throughput injected from the flowmeter and q is the throughput into the first chamber of the dynamic expansion system. We compare the signals from SRG1 with the gate valve between the flow splitter and the diverter chamber in the open and closed states. From Eq. (35) it follows that

$$p_{1,\text{open}} = \frac{r_{\text{p}}}{r_{\text{p}} - 1} \frac{1}{C_0} \alpha q_{\text{FM}}$$
 (37)

and

$$p_{1,\text{closed}} = \frac{r_{\text{p}}}{r_{\text{p}} - 1} \frac{1}{C_0} q_{\text{FM}}$$
 (38)

for these two states of the gate valve. Dividing these equations leads to

$$\frac{p_{1,\text{open}}}{p_{1,\text{closed}}} = \alpha \,. \tag{39}$$

The flow splitter is designed for $\alpha = 0.01$, using $\alpha \approx C_{\rm DE}/C_{\rm DC} = d_{\rm DE}^2/d_{\rm DC}^2$, where $d_{\rm DE} \approx 1$ mm and



FIG. 5. Schematic of the flow splitter connected to a diverter chamber and our dynamic expansion system. Quantities q, $q_{\rm FM}$, and $q_{\rm DC}$ with blue arrows are various gas throughputs. Blue arrows with thicker lines correspond to larger throughputs. Coefficients $C_{\rm DC}$ and $C_{\rm DE}$ are conductances of orifices connecting various chambers to the flow splitter. The gate value is used to measure ratio $q/q_{\rm FM}$. Pressures p_1 and p_2 ; gauges SRG1 and SRG2; valves V1 and V2; and conductance C_0 are defined as in Fig. 4.

 $d_{\rm DC} \approx 10 \text{ mm}$ are the diameters of the orifices of the conductances C_i . The length of the two orifices are identical.

D. Generating low flow with a XHV flowmeter

We require a flowmeter capable of generating flows between 2×10^{-13} mol/s and 10^{-9} mol/s and measuring these flows with a relative uncertainty better than 1%. Such flows will generate pressures between 2×10^{-11} Pa and 1×10^{-5} Pa in our dynamic expansion system. Moreover, we want this flow to be measured in a gasspecies independent way. To this end, we constructed an extreme-high-vacuum flowmeter (XHVFM) based on designs for a hydraulic constant-pressure flowmeter developed at NIST in 1987.⁷⁶

Constant-pressure flowmeters generate a flow $\dot{n}_{\rm FM}$ by allowing small amounts of gas to leak out of a variable volume, typically a vacuum bellows. This flow is measured as follows. As gas leaks out of the variable volume, its pressure $p_{\rm VV}$ would ordinarily decrease, but a feedback system keeps the pressure constant by decreasing the volume of the variable volume. Thus, the measurement equation for $\dot{n}_{\rm FM}$ becomes

$$\dot{n}_{\rm FM} = -\frac{p_{\rm VV}V_{\rm VV}}{RT_{\rm VV}} + \dot{n}_{\rm OG} \,, \tag{40}$$

derived from differentiating the ideal gas law with respect to time. Here, the rate of change of volume $V_{\rm VV} < 0$ can be measured accurately. Equation (40) includes outgassing from the walls of the variable volume with flow

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 $\dot{n}_{\rm OG} = Q_i A_{\rm VV}/RT_{\rm VV}$ with specific outgassing rate per unit surface area, Q_i , of species *i*, presumably H₂, and combined surface area $A_{\rm VV}$. We note that measurements of $T_{\rm VV}$ and $\dot{V}_{\rm VV}$ are gas-species independent, and $p_{\rm VV}$ is measured using gauges that do not dependent on gas species.

The volume of the variable volume can be changed with one of several techniques. Perhaps the simplest is to plunge a piston into the volume.⁷⁶ Because of leaks past the sliding seal, however, this limits flows to $> 10^{-8}$ mol/s. The technique most often used at NIST relies on flexible vacuum components, like vacuum bellows, held in canisters filled with pressurized oil.⁷⁶ When a piston is plunged into the oil, the hydraulic oil compresses the bellows. If the oil is incompressible, the change in the volume of the piston protruding into the oil is equal to the change in the volume of the bellows. A third technique is to eliminate the oil and calibrate a change in the volume of the bellows with a known linear displacement.^{16,17,77,78} We use the hydraulic technique, described in detail in Sec. III D 1.

To achieve a relative uncertainty of less than 1% in $\dot{n}_{\rm FM}$ for flows as low as 1×10^{-13} mol/s, we made several improvements to the original design, which can only achieve a 1% uncertainty for flows larger than about 1×10^{-11} mol/s. In the new design, the fill pressure of the variable volume is still constrained to lie between 13 Pa and 133 kPa, where absolute pressure gauges and transfer standards, like capacitance diaphragm gauges and resonant silicon gauges, can measure p_{VV} well. Consequently, the conductance of the leak $C_{\rm L}$ had to be decreased by a factor of 100, and the lowest available rate of change of volume $V_{\rm VV}$ had to be decreased by the same factor. This constraint on $V_{\rm VV}$ follows immediately from equating $\dot{n}_{\rm FM} = p_{\rm VV}C_{\rm L}/RT_{\rm VV}$ and Eq. (40) for negligible outgassing rates. Finally, we needed to decrease outgassing from the walls of the variable volume, that is $\dot{n}_{\rm OG}$ in Eq. (40), by careful baking. The baking procedures are described in Sec. III A; we routinely measure $\dot{n}_{\rm OG} < 10^{-15}$ mol/s as described in Sec. III D 2. In the end, the type-B uncertainty of $u(\dot{n}_{\rm FM})/\dot{n}_{\rm FM}$ is < 0.2 % over its entire operating range; the corresponding type-A uncertainty is approximately 1 % at 10^{-13} mol/s and drops to below 0.1 % for flows > 10^{-12} mol/s.

The plumbing diagram for the XHVFM is shown in Fig. 6. The XHVFM has four parts: a fill system for predictably adding gas, an evacuation system for removing gas, a fixed-leak (FL) flowmeter, and a variable-leak (VL) flowmeter. Only one flowmeter is used at a time. The unused flowmeter is sealed off during operation. The FL and VL flowmeters have a fixed and a variable leak, respectively, through which gas from their variable volume flows to the output port. The fixed leak is a standard conductance element (SCE),⁷⁹ while the variable leak is an all-metal vacuum flow control valve (MKS 245). The variable volumes of the FL and VL flowmeters are connected to a shared reference volume. The temperature of each variable volume is measured using two platinum



FIG. 6. Plumbing diagram of the extreme-high vacuum flowmeter. The transparent colored regions define the four, partly overlapping components of the flowmeter as described in the text. The "output" of the flowmeter connects to our flow splitter and dynamic expansion system (not shown). The pressures in variable volumes FLVV and VLVV, each enclosed in a canister with oil (blue areas), are determined by first measuring pressure differentials (with two Δp gauges) with gas in a reference volume (RV). The pistons in the oil canisters are used to change the volume of the variable volumes. The pressure in the reference volume is measured by absolute gauges (connected at "to absolute p gauge(s)"). Opening and closing of the many pneumatically-controlled valves determines which volumes and tubings (black lines) of the flowmeter are connected for evacuation with the pumps or filling from the gas cylinder or ballast volume. Other abbreviations: FLVV: fixed-leak variable volume; VLVV: variable leak variable volume; SCE: standard conductance element; TC gauge: thermocouple gauge; WR gauge: wide range cold-cathode/Pirani gauge; and CC: crimped capillary.

resistance thermometers mounted to the side of the oil canister surrounding the variable volume. The hydraulic systems controlling the piston and bellows as well as the air-bubble-free loading of the oil into the canister are described in Sec. III D 1. Gas flow from a fixed leak is more stable and more reliable at lower flows than that of a variable leak. Hence, we use the fixed leak for all results shown in this paper.

We do not measure pressures in a variable volume directly. Instead its pressure $p_{\rm VV}$ is compared against the pressure $p_{\rm RV}$ in a reference volume of ≈ 200 mL, which is installed in parallel to the variable volume, using a differential capacitance diaphragm gauge (CDG). Under proper flowmeter operating conditions the gauge will measure null corresponding to $p_{\rm VV} = p_{\rm RV}$. We utilize dif-

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ferential CDGs that operate at pressures below 133 Pa. No gas passes through such gauges. This design has two advantages. First, differential pressures can often be measured with greater precision than absolute pressures, which consequently reduces noise in the feedback loop to maintain a constant pressure. Second, the flowmeter's large operating range requires the use of multiple absolute pressure gauges to measure pressure in the reference volume. These absolute pressure gauges have a combined volume that is non-negligible, sometimes as large as 50%of that of the reference volume. Using differential pressure measurements then enables us to use a volume for the variable volume that is small compared to that of the reference volume and, simultaneously, to maintain pressure changes for a given displacement volume of the piston that are as large as when the gas volume in the absolute gauges were negligible. We use bakeable CDGs, described in Sec. IIID3 and Ref. 80, to measure the absolute pressure $p_{\rm RV}$ in the reference volume.

The flowmeter must first be filled to the appropriate pressure to generate flow $\dot{n}_{\rm FM}$. This process fills the ballast and reference volumes as well as the variable volume with the piston set at its default or initial position with the same gas to the same pressure. Details are found in Sec. IIID4. Once filled, the valves connecting the variable and reference volumes to the rest of the XHVFM are closed and flow measurements commence by careful movement of the piston. These measurements are described in Ref. 81, but a brief synopsis is given in Sec. IIID 5. Once a flow measurement is finished, the piston is reset to its initial position and gas lost from the variable volume is replenished by connecting the variable and reference volumes to the large 6.4 L ballast volume by opening the relevant values. The flow measurement can then be repeated, or the XHVFM filled to a higher pressure to increase $\dot{n}_{\rm FM}$, or, evacuated to a lower pressure to decrease $\dot{n}_{\rm FM}$. When flow measurements are completed, the XHVFM is typically evacuated and maintained at its base pressure of $< 10^{-5}$ Pa. Evacuation is handled by the evacuation system described in Sec. IIID6.

1. Oil-based hydraulic system for the variable volumes

The approximately 14 mL variable volume of the fixedleak flowmeter is surrounded by an oil-containing canister as schematically shown in Fig. 7. The bellows portion of this variable volume has a volume that is less than 3 mL. The remainder of the volume corresponds to the volume of connecting plumbing, the differential pressure gauge, and other components. The volume of the oil in the canister is 8(1) mL, measured gravimetrically using ethanol.

The pressure in the oil must be maintained at pressures greater than atmospheric pressure in order to prevent drawing in of air bubbles into the oil from leak seals and fittings in the canister. Such bubbles would prevent displacements of the piston from creating equal but



FIG. 7. A schematic of the fixed-leak variable volume and its associated oil-based hydraulic system. The acceleration of earth's gravity is pointing downwards. Pink regions denote gas in the variable volume and blue regions denote hydraulic oil. Dark gray, light gray, and hashed components are made of titanium, stainless steel, and aluminum, respectively. The upper and lower valves are used to evacuate, fill, and repressurize the hydraulic system with oil. The following abbreviations are used: Δp : differential pressure gauge, BV: ballast volume, RV: reference volume, and SCE: standard conductance element. These components also correspond to those used in Fig. 6.

opposite changes in the volume of the variable volume, rendering measurement of $V_{\rm VV}$ impossible. The pressure differential between the inside and outside of the bellows will thus be greater than 1 atm, enough to cause the bellows to collapse. A spring with spring constant 80 N/cm inside the variable volume prevents this collapse.

A 10 cm long, 3.1749(5) mm diameter steel piston is plunged into the oil through a Viton o-ring seal. The change in the linear position of the piston is precisely controlled using a micrometer screw with a displacement rate of 0.499(1) mm/turn. In our setup, the displacement volume for the piston, ΔV_{piston} , is always less than 0.25 mL. We measure ΔV_{piston} relative to the maximal insertion of the piston into the oil canister allowed by our assembly. Thus, $\Delta V_{\text{piston}} < 0.82$

The oil canister is connected to tubes and values that allow for the initial filling as well as the repressurization of the oil. As shown in Fig. 7, the upper valve connects to a vertically-aligned oil reservoir. Here, vertical is defined with respect to earth's gravity. This reservoir is used to re-pressurize the oil when appropriate and to measure the compressibility of the variable volume. The bottom valve connects to an oil source, a diffusion pump, for the initial fill of the system.

The canister must be filled with oil before the XHVFM

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can be made operational. This is a multi-step process. After initial assembly, all components of the XHVFM, even the canister, are filled with air at atmospheric pressure, and thus no pressure differential exists across the walls of the bellows. In this configuration, the spring pushes the bottom of the bellows into the bottom of the oil canister. The flowmeter is then evacuated, establishing a pressure difference across the walls of the bellows causing the spring and bellows to compress, lifting the bottom of the bellows from the bottom of the canister. Next, the air in the canister is removed with the help of a rough pump connected to the upper valve, temporarily replacing the oil reservoir. The air pressure is lowered to at most 10 Pa. The pressure differential across the walls of the bellows is thus again removed, and the spring pushes the bottom of the bellows into the bottom of the canister. In this configuration the path of both gas and oil would be blocked if not for a small notch in the floor allowing flow around the bottom of the bellows.

We must remove air bubbles and dissolved gas from the oil, Santovac 5, before we can push the oil into the canister. These imperfections would increase the compressibility of the oil. The removal of bubbles and dissolved gases is achieved by baking approximately 200 mL of oil under vacuum above its boiling point in the diffusion pump for six hours. In this configuration the diffusion pump is not used as a pump, but only used as a heater. Subsequently, the diffusion pump is back filled with approximately 150 kPa of argon gas. The drain line of the diffusion pump is then connected to the lower valve of the oil canister and this final plumbing connection is evacuated of air using the rough pump. Afterwards the drain value on the diffusion pump is opened, starting the flow of oil from the diffusion pump filling the canister from the bottom up. After the canister is filled and oil appears in transparent PVC tubing that connects the upper valve to the rough pump, this valve is closed and the rough pump is turned off and disconnected.

To verify that no bubbles are trapped in the oil in the canister, the upper valve is reopened and oil coming out of the valve is collected and monitored for the presence of bubbles. If bubbles are seen, the flow is allowed to continue until no more bubbles appear. Once the oil is determined to be bubble free, generally after the flow of 20 mL of additional oil, the upper valve is closed and the reservoir attached. The upper valve is then opened one last time to allow 10 mL of oil to fill the reservoir. Then the upper valve is closed, followed by the lower valve, and the tubing connecting to the diffusion pump removed. This process leaves bubble-free oil in the canister, pressurized at the approximately 150 kPa backing pressure of the diffusion pump.

The reservoir system shown in Fig. 7 allows us to change the pressure of the oil. By attaching a regulated cylinder with gas at the desired pressure to the top of the reservoir, we can pressurize the oil in the canister by opening the upper valve, waiting for the oil in the canister and the reservoir to come to equilibrium, and closing the valve again. When oil is under pressure and the valve is closed, the spring in the bellows maintains that pressure, unless the compressibility of the oil changes or there is a leak. We find that we must periodically re-pressurize the oil. Because the bellows can only contract by at most 3 mL, the 10 mL oil in the reservoir is sufficient for our purposes.

During operation of the flowmeter, a finite change of volume of the piston into the oil canister, ΔV_{piston} , affects a change in the oil pressure, Δp_{oil} , and, in turn, a change of volume of the variable volume ΔV_{VV} . Specifically, we have

$$\Delta V_{\text{piston}} = \left[\left(\frac{\mathrm{d}V}{\mathrm{d}p} \right)_{\text{VV}} + \left(\frac{\mathrm{d}V}{\mathrm{d}p} \right)_{\text{oil}} \right] \Delta p_{\text{oil}}, \qquad (41)$$

where derivatives $(dV/dp)_j$ set the response of volume j = VV or "oil" to an infinitesimal increase in the oil pressure p_{oil} . Then

$$\Delta V_{\rm VV} \equiv -\left(\frac{\mathrm{d}V}{\mathrm{d}p}\right)_{\rm VV} \Delta p_{\rm oil} = -\frac{\Delta V_{\rm piston}}{1 + \left(\frac{\mathrm{d}V}{\mathrm{d}p}\right)_{\rm oil} / \left(\frac{\mathrm{d}V}{\mathrm{d}p}\right)_{\rm VV}} \tag{42}$$

We have measured $(dV/dp)_{VV}$ and $(dV/dp)_{oil}$ for the fixed-leak flowmeter. In fact, we have determined $(dV/dp)_{VV}$ by measuring the "dead" volume V_0 of the variable volume when $\Delta V_{\text{piston}} = 0$ as a function of p_{oil} . For this measurement, we set the oil pressure to p_{oil} , fill the variable volume with an initial n_0 moles of gas, and then close the input valve to the variable volume defining time t = 0. We then modulate the volume of the variable volume as $V_{VV}(t) = V_0 + \Delta V_{VV}(t)$, where $\Delta V_{VV}(t) \ge 0$ and $\Delta V_{VV}(t) \ll V_0$, so that pressure $p_{VV}(t)$ is given by

$$p_{\rm VV}(t) = \frac{n_{\rm VV}(t)RT_{\rm VV}}{V_0 + \Delta V_{\rm VV}(t)}, \qquad (43)$$

where $n_{\rm VV}(t) = n_0 - (\dot{n}_{\rm FM} - \dot{n}_{\rm OG})t$ is the number of gas molecules (in mol) at time *t*, time-independent $\dot{n}_{\rm FM}$ is the flow out of the variable volume through the fixed leak into the flowsplitter, and $\dot{n}_{\rm OG}$ is the constant flow from outgassing from the walls of the variable volume.

A measurement of $p_{\rm VV}(t)$ in response to a known triangle-wave modulation of the displacement volume of the piston $\Delta V_{\rm piston}$ is shown in Fig. 8(a). Assuming incompressible oil so that $\Delta V_{\rm VV} = -\Delta V_{\rm piston}$ (as we shall see, this assumption is valid at the level of uncertainty of this measurement), we fit the recorded trace of $p_{\rm VV}(t)$ to Eq. (43) using the known $\Delta V_{\rm piston}(t)$ and $T_{\rm VV}$ with n_0 , V_0 , and $\dot{n}_{\rm FM} - \dot{n}_{\rm OG}$ as fit parameters. The fit yields a value $V_0 = 13.28(7)$ mL. The uncertainty is dominated by the uncertainty in the differential pressure measurement, which is itself dominated by calibration errors. Figure 8(b) shows similar measurements of V_0 as a function of oil pressure $p_{\rm oil}$. A linear fit to this data finds $(dV/dp)_{\rm VV} = -9.7(5) \times 10^{-3} \text{ mL/kPa}.$

Next, we turn our attention to the measurement of $(dV/dp)_{oil}$ or, equivalently, V_{oil}/B , where B is the bulk modulus of oil. We use a separate apparatus consisting of

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FIG. 8. Measurement of the dead volume V_0 and compressibility of the variable volume of the fixed-leak flowmeter. Panel (a) shows the absolute pressure in the variable volume $p_{\rm VV}$ as a function of time t by changing its volume with the piston. For this data $p_{\rm oil} = 150\,$ kPa. Blue points are data. The orange curve is a fit. (b) Dead volume V_0 (blue points) extracted from data such as that shown in panel (a) as a function of oil pressure $p_{\rm oil}$ with a linear fit to obtain the compressibility $(dV/dp)_{\rm VV}$ of the variable volume (solid line). Error bars represent the total standard k = 1 uncertainty. The statistical, type-A uncertainty is approximately the size of the points. Reproduced from S. Eckel, D. S. Barker, J. Fedchak, E. Newsome, J. Scherschligt, and R. Vest, Metrologia **59**, 045014 (2022), public domain.

canister with an identical piston and micrometer screw, but without a variable volume. The volume of oil inside the canister is 103(1) mL. This apparatus is filled with oil in an manner identical to that for the flowmeter. The piston was displaced and a pressure rise is recorded with the pressure gauge attached to the canister. A linear fit of the pressure as function of the piston displacement yields bulk modulus B = 1.4(3) GPa.

Combining our values for $(dV/dp)_{VV}$ and $(dV/dp)_{oil}$ we find $\Delta V_{VV} = -[1 - 5.8(1.2) \times 10^{-4}]\Delta V_{piston}$. This correction is smaller than the uncertainty in the measurement of V_0 , justifying our earlier assumption that the oil is incompressible. For the measurement of flow, described in Sec. III D 5, we use this relationship in Eq. (40).

2. Outgassing and bakeability

Low outgassing rates from surfaces in the flowmeter are just as important as those in the dynamic expansion



FIG. 9. Rate-of-rise measurement of outgassing in an isolated fixed-leak variable volume at a temperature of 299.10(3) K. Blue points are measured pressure differences of the differential CDG between the variable and reference volumes as function of time. The green points are 10 min measurements of the offset pressure and drift of the differential gauge. The orange line is a linear fit to the blue data points and determines the pressure rate of rise. Reproduced from S. Eckel, D. S. Barker, J. Fedchak, E. Newsome, J. Scherschligt, and R. Vest, Metrologia **59**, 045014 (2022), public domain.

system described in Sec. III A. Here, we again achieve low outgassing by removing hydrogen before assembly and removing water after assembly. To further minimize H_2 outgassing in the flowmeter, we use titanium vacuum parts where possible. Stainless steel parts are pre-treated inside our home built vacuum furnace according to the procedure outlined in Sec. III A. To remove desorbed water from surfaces, we bake the assembled flowmeter at approximately 110 °C for two to three days. Water can be a contaminant in gases entered into the flowmeter so that after several fill procedures non-negligible amounts of water can re-adsorb to the walls. For this reason, we have designed the flowmeter to facilitate repeated 150 °C bakes: it is contained in an insulated box with permanently-installed cartridge heaters.

For the optimal operation of the flowmeter, it is important to characterize the residual outgassing flow, $\dot{n}_{\rm OG}$ in Eq. (40), inside the variable volume. We use a rate-ofrise technique to measure \dot{n}_{OG} . Figure 9 shows a typical 6 h measurement of the pressure difference Δp between an isolated fixed-leak variable volume and the reference volume, both at a temperature of $T_{\rm VV} = 299.10(3) \, {\rm K}$. The input valve to the variable volume is closed, and the reference volume continues to evacuate through the turbo pump, ensuring a $p_{\rm RV} < 10^{-4}$ Pa. The output valve of the variable volume remains open and gas will leak out into the flowsplitter and dynamical expansion system. The maximum pressure differential across the leak, however, is small at < 5 mPa, and consequently the flow out of the variable volume is $< 10^{-16}$ mol/s and is therefore negligible.

Differential capacitance diaphragm gauges do not have a well-defined zero offset, *i.e.*, they show a non-zero pressure differential even when the actual pressure differential is zero. This offset can be large and change with time as environmental conditions like temperature and humidity change. The data in Fig. 9 shows such an offset. It is



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FIG. 10. Three bakeable capacitance diaphragm gauges (fuchsia cylinders) housed inside a temperature controlled box (semi-transparent beige). The unit for temperature control near room temperature (purple) protrudes from the left side of the box. Reproduced from J. Scherschligt, D. Barker, S. Eckel, J. Fedchak, and E. Newsome, Vaccum 197, 110801 (2022), public domain.

36.5(5) mPa and drifts at a rate of $-0.5(1.0) \times 10^{-9}$ Pa/s. This offset and drift is determined by recording Δp when all connecting valves are open and the pressures of the two volumes are in equilibrium. These values of Δp are recorded for 10 min before and after the 6 h rate-of-rise measurement.

A fit to the data in Fig. 9 gives rate of pressure rise s, corrected for the pressure offset and drift, during the 6 h outgassing measurement. We then derive that $\dot{n}_{\rm OG} = sV_{\rm VV}/RT_{\rm VV} = 9.6(9) \times 10^{-16}$ mol/s. The uncertainty of $\dot{n}_{\rm OG}$ is dominated by statistics: the short-term repeatability is about 10%. This outgassing rate is a factor of 100 better than that of our previous best standard flowmeter at NIST.

3. Absolute pressure gauges

Three capacitance diaphragm gauges (CDGs) are attached to the reference volume and measure its absolute pressure between 10 Pa to 100 kPa of interest to our flowmeter. A computer-aided design (CAD) drawing of these three gauges with their housing and plumbing is shown in Fig. 10. We use three series 616A Baratron gauges, produced by MKS instruments,⁸³ with nominal upper pressure limits of 133 Pa, 1.33 kPa, and 133 kPa, respectively. Specified to be bakeable up to at least 400 °C and operable up to at least 300 °C, the CDGs are attached to the flowmeter and housed in a temperaturecontrolled box, which enables low-temperature in situ baking without the need for special equipment. They were baked at 450 °C for 30 days to remove hydrogen

dissolved in the walls of the gauges before being tested or installed on the flowmeter.

Unlike other CDGs used at NIST,⁸⁴ however, the three gauges did not have their long-term stability characterized, and thus their uncertainty budget was not well known. In Ref. 80, we determined their stability under a controlled series of bakes. We summarize the findings here. The pressure readings of the three bakeable CDGs are compared to pressure reading of a NIST transfer standard. The NIST transfer standard is also comprised of a set of CDGs maintained in a temperature-stabilized enclosure, but the transfer-standard gauges have been calibrated using the NIST primary laboratory standard for pressure, the Ultrasonic Interferometer Manometer.

The transfer standard and bakeable CDGs are compared in the following manner. Both gauges are connected to the "to absolute p gauge(s)" port in Fig. 6 so that both measure the pressure in the reference volume $p_{\rm BV}$. Starting from $p_{\rm BV} = 0$ Pa, here at least three orders of magnitude less than 10 Pa, the flowmeter is filled (see Sec. III D 4) to a series of 27 pressure points, collectively called a run, that sampled the 10 Pa to 10 kPa pressure range. A few of the pressure points were accessible to or measurable by more than one of the three CDGs, but generally there is little overlap. For each of the three CDGs, the relevant (r_{CDG}, p_{RV}) data of each run are fit to cubic polynomial

$$p_{\rm RV} = c_0 + c_1 r_{\rm CDG} + c_2 r_{\rm CDG}^2 + c_3 r_{\rm CDG}^3 , \qquad (44)$$

where r_{CDG} is the pressure reading of the bakeable CDG and $p_{\rm RV}$ is the pressure in the reference volume as determined by the NIST transfer standard. The four c_i are fit parameters. Under ideal conditions $c_1 = 1$, while all other coefficients are zero. About ten runs were carried out before baking at 110 °C for roughy 72 hours and cooling back down to room temperature. This process was repeated for a total of six cycles of nine or ten runs and one bake, followed by ten runs after the final cool down. The complete process took about three months.

Coefficients c_0 and c_1 as functions of run number 0 to 70 are shown in Figs. 11 and 12, respectively. Bakes are also indicated. A panel in these figures corresponds to data for one of the three bakeable CDGs. We immediately observe that c_1 is close to one as expected with the biggest, 15% discrepancy for the bakeable CDG rated for pressures up to 133 kPa. Furthermore, the value of c_1 sometimes but not always jumps after a bake. Between bakes the value is more stable. Still, we conclude that once baked, *i.e.*, including data only after bake #1, the 90 % or two-sigma variation in c_1 is 0.08 %, 0.2 %, and 0.1 %. for the CDGs with an upper pressure limit of 133 Pa, 1.33 kPa, and 133 kPa, respectively.

The absolute values for zero-offset coefficient c_0 in Fig. 11 are about 0.2 Pa, 2 Pa, and 50 Pa for the CDGs with an upper pressure limit of 133 Pa, 1.33 kPa, and 133 kPa, respectively. Thus c_0 scales roughly as 10^{-4} times the upper pressure limit. The value of c_0 nearly always jumps after a bake and, in fact, changes by amounts

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FIG. 11. Expansion coefficients c_0 of the calibration of our three absolute pressure gauges as functions of run number for the gauges with upper pressure limit of 133 Pa, 1.33 kPa, and 133 kPa in the top, middle, and bottom panel, respectively. Vertical dashed lines denote bakes after every nine or ten runs. The statistical standard uncertainty of the coefficients is smaller than the points. Reproduced from J. Scherschligt, D. Barker, S. Eckel, J. Fedchak, and E. Newsome, Vaccum **197**, 110801 (2022), public domain.



FIG. 12. Expansion coefficients c_1 of the calibration of our three absolute pressure gauges as functions of run number for the gauges with upper pressure limit of 133 Pa, 1.33 kPa, and 133 kPa in the top, middle, and bottom panel, respectively. Vertical dashed lines denote bakes after every nine or ten runs. Uncertainty bars represent the k = 1 statistical uncertainty. For most data this uncertainty is smaller than the marker. Reproduced from J. Scherschligt, D. Barker, S. Eckel, J. Fedchak, and E. Newsome, Vaccum **197**, 110801 (2022), public domain.

on the order of its value. Between bakes the value for c_0 drifts with time.

The results suggest that the most accurate approach to measure pressure with the three CDGs must involve measuring the zero-order coefficient c_0 as often as possible, typically daily, but that we can re-use the linear and higher-order coefficients. The higher-order coefficients (not shown) have a similar behavior as c_1 . Luckily, it is quite simple to determine c_0 : one need only evacuate the flowmeter to its base pressure ($< 10^{-5}$ Pa) and measure $r_{\rm CDG} = -c_0$. Indeed this is recommended by the manufacturer as standard practice. So long as this procedure is carried out, the one-sigma reproducibility of the pressure readings of our baked CDGs is at worst 0.3%.

4. Filling

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The fill of the flowmeter also has multiple steps. First, if starting from an evacuated flowmeter, the valves connecting the flowmeter to the pumps are closed. From a gas cylinder, a desired atomic or molecular gas flows through a regulator and one or more of the three fixed crimped capillaries shown in Fig. 6 into the flowmeter by opening the relevant valves. The crimped capillaries have carefully chosen, distinct diameters and thus flows or throughputs. In fact, the three fixed leaks have calibrated throughputs of $q_{\rm in} = 520(40)$ Pa L/s, 4.9(3) Pa L/s, and 1.7(1) Pa L/s for nitrogen N₂, respectively, assuming an input pressure of 200 kPa from the regulator and a temperature of 23.4 °C. Gas slowly fills the ballast and ref-

erence volumes as well as one of the variable volumes. During the fill process, we only measure the pressure in the reference volume $p_{\rm RV}$.

Three typical fill curves of the reference volume with N_2 as function of time using the crimped capillary with throughput 4.9(3) Pa L/s are shown in Fig. 13(a). We start with an evacuated flowmeter with $p_{\rm BV} \approx 0$ Pa. At time t = 0 the value between the gas regulator and the crimped capillaries is opened. A pressure reading is taken approximately every 2 s. The three curves show similar behavior: the pressure initially increases rapidly before transitioning to a linear dependence with time. At stop time $t_{\rm S}$ when pressure $p_{\rm S}$ is reached, the valve controlling the fill is turned off. Subsequently, the pressure in the reference volume falls off exponentially to a final value $p_{\rm T}$ as the pressure in the system of volumes and connecting tubes equilibrates. These latter pressure transients are more clearly shown in an inset of Fig. 13(a). The data in this inset indicate that the pressure drop depends on the final pressure. Finally, we find from Fig. 13(a) as well as from fill trajectories using the other two crimped capillaries (not shown) that, after the initial transients in the first 20 s of the fill, the slopes $dp_{\rm RV}/dt$ for nitrogen are 69(2) Pa/s, 0.81(2) Pa/s, and 0.073(4) Pa/s for the three capillaries, respectively. Here, the uncertainties in parenthesis are only statistical.

We must understand the nature of the complicated fill curves of Fig. 13(a) because we wish to, as accurately as is possible, fill the flowmeter to pressure $p_{\rm T}$ to generate the desired flow $\dot{n}_{\rm FM} = p_{\rm T}C_{\rm L}/RT_{\rm VV}$. In particular, we

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FIG. 13. Typical N₂ gas fill trajectories and parameters of our XHV flowmeter. (a) Pressure in reference volume $p_{\rm RV}(t)$ as function of time t for three fill trajectories for N₂ using the crimped capillary with throughput 4.9(3) Pa L/s. All fills start near $p_{\rm RV} = 0$ Pa. Measured blue, orange, and green points follow fills with a target pressure $p_{\rm T}$ of 133 Pa, 400 Pa, and 1333 Pa, respectively. Black curves are the best fits to a non-linear conductance model described in the text. The upper left inset shows the electric circuit equivalent of this model. The lower right inset shows pressure differences $\Delta p(t) = p_{\rm BV}(t) - p_{\rm S}$ as functions of $\Delta t = t - t_{\rm S}$ after the fill was turned off at time $t = t_{\rm S}$ when $p_{\rm BV}(t_{\rm S}) = p_{\rm S}$. Colors are the same as in the main figure. (b) Pressure overshoot $p_{\rm O} = p_{\rm S} - p_{\rm T}$ as functions of target pressure $p_{\rm T}$ for the capillary with the smallest 1.7(1) PaL/s (green), middle 4.9(3)PaL/s (orange) and the largest 520(40) PaL/s throughputs (blue). Points are measurements, while solid curves are obtained from simultaneous fits to all data points using a linearized effective model for the conductances.

derive an analytical expression for the pressure overshoot in the reference volume. Then measurement of $p_{\rm RV}$, with relative uncertainty of less than 0.3% for our bakeable CDGs, is sufficient to trigger the stop of the fill and have the pressure in the flowmeter come to equilibrium such that

$$\frac{|p_{\rm RV}(t \to \infty) - p_{\rm T}|}{p_{\rm T}} < 0.03 .$$
 (45)

We model the flowmeter using the equivalent parallel-RC electrical circuit shown in the upper left inset of Fig. 13(a). In this circuit, the crimped capillaries become current sources with a "current" equal to throughput $q_{\rm in}$, volumes become capacitors, and conductances of constrictions, such as tubings, become "non-linear resistors." Pressures p_i at various points in the flowmeter become voltages in the circuit, where the electric ground corresponds to zero pressure. More precisely, volumes become circuit elements with throughput-pressure relation

$$q_j = V_j \frac{\mathrm{d}(p_j - p_i)}{\mathrm{d}t} \,, \tag{46}$$

where index j labels the volume of size V_j and p_j and p_i are absolute pressures on either side of the circuit element. Constrictions become circuit elements with non-linear throughput-pressure relation

$$q_j = [p_j - p_i] \times C_j([p_j + p_i]/2)$$
(47)

with pressure-dependent conductance function⁸⁵

$$C_j(\bar{p}) = \mathcal{C}_{0,j} + \mathcal{C}_{1,j}\bar{p}, \qquad (48)$$

where positive $C_{0,j}$ and $C_{1,j}$ are linear and non-linear conductances, respectively. When $C_{1,j} = 0$, coefficient $1/C_j$ is equivalent to the resistance of a resistor in an electric circuit. Equation (47) depends on the pressure difference $p_j - p_i$ across constriction j as expected for a resistor, but also on the absolute pressure $(p_j + p_i)/2$, to be interpreted as a typical, mean gas pressure in the constriction. The dependence on absolute pressure is unique to gas flow circuits and turns out to be crucial for a quantitative description of the later stages of a fill, where pressures are largest.

The throughput $q_{\rm in}$ from the crimped capillaries travels down two paths: one fills the reference volume via connecting tubes and one fills all other volumes, mainly the ballast volume, via corresponding connecting tubes. Analysis of the circuit diagram yields

$$q_{\rm in} = q_{\rm RV} + q_{\rm E} \tag{49}$$

from Kirkhoff's current rule with throughput through the path containing the reference volume

$$q_{\rm RV} = V_{\rm RV} \frac{\mathrm{d}p_{\rm RV}}{\mathrm{d}t} = (p_{\rm J} - p_{\rm RV})C_{\rm RV}([p_{\rm J} + p_{\rm RV}]/2) \quad (50)$$

and throughput through the path containing the other volumes

$$q_{\rm E} = V_{\rm E} \frac{\mathrm{d}p_{\rm E}}{\mathrm{d}t} = (p_{\rm J} - p_{\rm E})C_{\rm E}([p_{\rm J} + p_{\rm E}]/2).$$
 (51)

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is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0120500 Pressures $p_{\rm J}$, $p_{\rm RV}$, and $p_{\rm E}$ are defined in Fig. 13(a). By inserting the last of the equalities in Eqs. (50) and (51)into Eq. (49), we find that pressure $p_{\rm J}$ is solely a function of $p_{\rm RV}$ and $p_{\rm E}$ and has no explicit time dependence. In fact, $p_{\rm J}$ is the positive root of a quadratic equation using the pressure dependence of the conductance functions $C_i(\bar{p})$. Hence, Eqs. (50) and (51) form two coupled non-linear first-order differential equations in $p_{\rm RV}$ and $p_{\rm E}$ that we solve with numerical methods.

We can get intuition about the time dependence of $p_{\rm RV}$ and $p_{\rm E}$ when $C_j(\bar{p}) = C_{j,\rm eff}$ for all pressures \bar{p} . That is, we assume that the (non-zero) mean pressure in the constrictions does not significantly change during the fill. Then $p_{\rm J} = (q_{\rm in} + p_{\rm RV}C_{\rm RV,eff} + p_{\rm E}C_{\rm E,eff})/(C_{\rm RV,eff} + C_{\rm E,eff})$ and the two coupled differential equations for $p_{\rm RV}$ and $p_{\rm E}$ are linear with constant coefficients. We derive the general solution

$$p_{\rm RV}(t) = \frac{q_{\rm in}}{V_{\rm tot}} t + \mathcal{P} + \frac{V_{\rm E}}{V_{\rm tot}} \left[p_{\rm ref} - \mathcal{Q}e^{-t/\tau} \right]$$
(52)

and

$$p_{\rm E}(t) = \frac{q_{\rm in}}{V_{\rm tot}} t + \mathcal{P} - \frac{V_{\rm RV}}{V_{\rm tot}} \left[p_{\rm ref} - \mathcal{Q}e^{-t/\tau} \right] , \qquad (53)$$

where pressure

$$p_{\rm ref} = \frac{q_{\rm in}}{V_{\rm tot}} \left(\tau_{\rm E} - \tau_{\rm RV} \right) \,, \tag{54}$$

total volume $V_{\text{tot}} = V_{\text{E}} + V_{\text{RV}}$, "RC" time constants $\tau_{\rm RV} = V_{\rm RV}/C_{\rm RV, eff}, \ \tau_{\rm E} = V_{\rm E}/C_{\rm E, eff}, \ {\rm and} \ \tau = V_{\mu}/C_{\mu, eff}$ with $1/C_{\mu,\text{eff}} = 1/C_{\text{E,eff}} + 1/C_{\text{RV,eff}}$ and $1/V_{\mu} = 1/V_{\text{E}} + 1/C_{\text{RV,eff}}$ $1/V_{\rm RV}$. The constants \mathcal{P} and \mathcal{Q} are determined by the initial conditions for $p_{\rm RV}$ and $p_{\rm E}$.

The initial conditions for the model are those from the experimental fill procedure. That is, at time t = 0 we have $p_{\rm RV} = p_{\rm E} = 0$. Between t = 0 and the stop time $t_{\rm S}$ the throughput $q_{\rm in} > 0$. At time $t = t_{\rm S}$, the fill is turned off or stopped so that for $t > t_{\rm S}$ throughput $q_{\rm in} = 0$. Then, for $t \in [0, t_{\rm S}]$, we easily realize that $\mathcal{P} = 0$ and $Q = p_{\rm ref}$ and define pressure $p_{\rm S} \equiv p_{\rm RV}(t_{\rm S})$ at the time that the fill stops. For $t > t_{\rm S}$, after some thought, we realize that both $p_{\rm RV}(t)$ and $p_{\rm E}(t)$ approach

$$p_{\rm T} = \frac{q_{\rm in}}{V_{\rm tot}} t_{\rm S} \tag{55}$$

for $t \to \infty$. Finally, the pressure drop or overshoot in the reference volume from $t = t_{\rm S}$ to $t \to \infty$ is

$$p_{\rm O} = p_{\rm S} - p_{\rm T} = \frac{V_{\rm E}}{V_{\rm tot}} p_{\rm ref} (1 - e^{-t_{\rm S}/\tau}) \,.$$
 (56)

and $p_{\rm J} \rightarrow p_{\rm T}$ for $t \rightarrow \infty$.

In practice, $V_{\rm RV} \ll V_{\rm E}$, $C_{\rm RV,eff} \approx C_{\rm E,eff}$, and $t_{\rm S} \gg \tau \approx$ $V_{\rm RV}/C_{\rm E,eff}$ so that the pressure overshoot is

$$p_{\rm O} \approx \frac{q_{\rm in}}{C_{\rm E,eff}} \,, \tag{57}$$

independent of the volumes V_i and stop time t_s . In this limit, we also realize that $p_{\rm O} \ll p_{\rm T}$ when $t_{\rm S} \gg \tau_{\rm E} \approx$ $(V_{\rm E}/V_{\rm RV})\tau$, which might not always be fulfilled for small stop times $t_{\rm S}$.

We find that the solution in Eq. (52) qualitatively resembles the three traces in Fig. 13(a). The pressure in the reference volume initially increases rapidly before transitioning to a linear curve with slope $q_{\rm in}/V_{\rm tot}$. After the flow is stopped, this pressure drops exponentially to its asymptotic and target value. Note that the fitted $q_{\rm in}/V_{\rm tot}$ from Fig. 13(a) agrees to within 10% with the calibrated throughput of the crimped capillary and our measured $V_{\text{tot}} = 6.4 \,\text{L} + 0.2 \,\text{L} = 6.6 \,\text{L}$, the sum of the ballast and reference volumes.

In the linear model of the fill, the exponential pressure rise at the beginning and fall at the end of the fill procedure are symmetric so that the long-time or target pressure is simply $p_{\rm T} = q_{\rm in} t_{\rm S} / V_{\rm tot}$. In fact, for $t_{\rm S} \gg \tau$ the pressure overshoot $p_{\rm S} - p_{\rm T}$ in the reference volume is independent of the stop time. This is not true for the experimental data shown in an inset of Fig. 13(a). The overshoot increases with $t_{\rm S}$ and thus with $p_{\rm T}$. To achieve the observed asymmetric rise/fall, we must include the non-linear conductance of the distribution tubing in Eqs. (47) and (48).

The black curves in Fig. 13(a) show best fits to the data from $t \in [0,\infty]$ using a non-linear conductance. These curves are numerical solutions of the differential equations in Eqs. (49), (50), and (51) and replicate the data quantitatively. For these non-linear least-squares fits, it turns out to be convenient to use $q_{\rm in}/V_{\rm tot}$, $V_{\rm RV}/V_{\rm tot}$, $\mathcal{C}_{0,\mathrm{RV}}/V_{\mathrm{tot}}, \mathcal{C}_{1,\mathrm{RV}}/V_{\mathrm{tot}}, \mathcal{C}_{0,\mathrm{E}}/V_{\mathrm{tot}}, \text{ and } \mathcal{C}_{1,\mathrm{E}}/V_{\mathrm{tot}} \text{ as the six}$ independent fit parameters.

In practice, we record $p_{\rm RV}(t)$ during the fill but we can not afford to fit in real time each fill in as much detail as in Fig. 13(a). Instead, we calculate from the required target pressure $p_{\rm T}$ and the modeled overshoot $p_{\rm O}$ a stop pressure $p_{\rm S} = p_{\rm T} + p_{\rm O}$, such that when $p_{\rm BV}(t) > p_{\rm S}$ during the fill, the upstream and downstream valves of the capillaries are closed and the fill stops. This also defines stop time $t_{\rm S}$. We record $p_{\rm RV}(t)$ for times $t \le t_{\rm S} + 5\tau$.

We calibrate the model of the overshoot by measuring six or seven values of $p_{\rm O} = p_{\rm S} - p_{\rm RV}(t \to \infty)$ as a function of $p_{\rm RV}(t \to \infty)$ for each capillary, spanning a target pressure range between 10 Pa and 10 kPa in the reference volume. This data as a scatter plot of $p_{\rm O}$ versus $p_{\rm RV}(t \to \infty)$ is shown in Fig. 13(b). We model the data in Fig. 13(b) by linearizing the conduction function in Eq. (47) assuming that the pressure drop in the reference volume is small compared to the target pressure and compute the conductance functions $C_i(\bar{p})$ at pressure

$$\bar{p} = \frac{p_{\rm J} + p_j}{2} \bigg|_{t \to \infty} = p_{\rm T} \,, \tag{58}$$

which is the same for j = RV and E. For our flowmeter with $V_{\rm RV} \ll V_{\rm E}$ and $C_{\rm RV}(p_{\rm T}) \approx C_{\rm E}(p_{\rm T})$, we derive

$$p_{\rm O} \approx \frac{q_{\rm in}}{\mathcal{C}_{0,\rm E} + \mathcal{C}_{1,\rm E}\,\bar{p}} = \frac{q_{\rm in}}{V_{\rm tot}} \frac{V_{\rm tot}}{\mathcal{C}_{0,\rm E} + \mathcal{C}_{1,\rm E}\,p_{\rm T}} \tag{59}$$

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as a qualitatively correct analysis of the $q_{\rm in}$ and $p_{\rm T}$ dependence of the pressure overshoot.

This analysis suggests the following two step fit procedure of the experimental data in Fig. 13(b). First, for each capillary c we determine $\Phi_c = q_{\rm in}/V_{\rm tot}$ and uncertainty $u(\Phi_c)$ from the six or seven measured ratios $p_{\rm T}/t_{\rm S}$ and Eq. (55). Second, we fit the three dimensional data set $(\Phi_c, p_{\rm T}, p_{\rm O})$ to

$$p_{\rm O} = \Phi_c \frac{\tau_0}{1 + p_{\rm T,c}/p_{\rm NL}} \tag{60}$$

with the restriction that target pressure $p_{\mathrm{T},c}$ is one of the p_{T} measured with capillary c. Then the coefficients τ_0 and p_{NL} are fit parameters shared across all capillaries. This fit is shown in Fig. 13(b), and replicates the observed data well. From the fit we also find that nonlinear conductance effects are important for target pressures larger than $p_{\mathrm{NL}} = 520(140)$ Pa.

The residuals between the small set of measured $p_{\rm O}$ and corresponding fitted $p_{\rm O}$ in Fig. 13(b) are a measure of our fill accuracy. For target pressures $p_{\rm T} > 200$ Pa, this leads to fractional differences $|p_{\rm O,measured} - p_{\rm O,modeled}|/p_{\rm T} < 1$ %. While this suggests that we can set the pressure in the flowmeter to within 1% in this pressure range, in practice this procedure is slightly less accurate: generally working to within 3%, because of flow variations in the capillaries on much longer time scales than shown in Fig. 13(a). The fit also shows that target pressures below 200 Pa should not be created with the mid-sized capillary with its throughput of 4.9(3) Pa L/s; likewise, target pressures below 2.5 kPa should not be created with the large-sized capillary with throughput 520(40) Pa L/s. In these cases, discrepancies of $|p_{O,\text{measured}} - p_{O,\text{modeled}}|/p_{T} > 1$ %, and smaller discrepancies can be achieved with the smaller capillaries at the expense of longer fill times $t_{\rm S}$.

For target pressures $p_{\rm T} < 200$ Pa and using the capillary with the smallest throughput of 1.7(1) Pa L/s, the pressure overshoot can be significant compared to the target pressure. In this regime, the nonlinear effects of the conductances are small and τ can be as large as 400 s due to the small value of $C_{0,\rm E}$. As a result, $t_{\rm S} \lesssim \tau$, and thus Eq. (56) should be used. Nevertheless, we find fit results with Eq. (60) are sufficiently accurate that fractional differences no larger than $|p_{\rm O,measured} - p_{\rm O,modeled}|/p_{\rm T} < 25$ % at $p_{\rm T} = 25$ Pa and falling to 1 % at 120 Pa are observed. For the CAVS, this does not pose a problem as we ordinarily operate with fill pressures $p_{\rm T} > 100$ Pa.

We note that the procedure of triggering on $p_{\rm S}$ and modeling $p_{\rm O}$ also works for fills that start at non-zero pressure in the reference volume, provided that $t_{\rm S} \gg \tau$. In principle, we need to determine Φ_c , α_0 and α_1 for the different gases used in the flowmeter. In practice, when changing gases, we measure the Φ_c in Eq. (59) for the new gas species and scale α_0 and α_1 according to $1/\sqrt{m}$, the expected scaling of conductance coefficients $C_{i,E}$.⁸⁵

5. Flow measurement

We have extensively tested and quantified the uncertainty budget of the flow $\dot{n}_{\rm FM}$ or throughput $q = \dot{n}_{\rm FM} R T_{\rm VV}$ out of flowmeter using the variable volume with the fixed leak. Details are described in Ref. 81. Here, we only give a brief synopsis.

The procedure for measuring flow or throughput out of the flow meter is as follows. The flow meter is first filled to the correct target pressure $p_{\rm RV}$ in the reference volume that produces the desired flow, as in Sec. III D 4. The zero offset of the differential gauge, described in Sec. III D 2, is measured with the pressure in the variable and reference volumes in equilibrium, *i.e.*, with the connecting values between these volumes open.

Next, the values connecting the variable, reference, and ballast volumes are closed. Closing these valves freezes or fixes the amount of gas in the reference volume; outgassing flux in the reference is negligible during the measurement. A software proportional-integratordifferentiator (PID) then adjusts the piston's velocity to keep the pressure difference between the variable and reference volumes $\Delta p = p_{\rm VV} - p_{\rm RV}$ as close to zero as possible, while gas leaves the flowmeter through the fixed leak. Once the piston's volume displacement rate V_{piston} stabilizes, *i.e.* is time independent, and $\Delta p = 0$, the flow *measurement* is stable and the software begins to record the nominally constant pressure in the reference volume $p_{\rm RV}$, temperature $T_{\rm VV}$, pressure difference Δp , and piston as well as changing piston position, every 5 seconds. The beginning of this record is defined as t = 0. The piston's displacement $\Delta V_{\text{piston}}(t)$ relative to its fully inserted position determines $V_{\rm VV}(t)$ through $V_{\rm VV}(t) = V_0 - (1 - \epsilon) \Delta V_{\rm piston}(t)$, using the results $V_0 = 13.28(7)$ mL and $\epsilon = 5.8(1.2) \times 10^{-4}$ from Sec. III D 1.

The flow $\dot{n}_{\rm FM}$ and its statistical (type-A) uncertainty is determined from this record by first constructing $n_{\rm VV}(t)$, where $n_{\rm VV}(t) = p_{\rm VV}(t)V_{\rm VV}(t)/RT_{\rm VV}(t)$ as a function of time and then fitting slope $\dot{n}_{\rm VV}$. Minus one times this slope is the first term in Eq. (40). Here, the pressure in the variable volume is $p_{\rm VV}(t) = p_{\rm RV}(t) + \Delta p(t)$. This procedure naturally accounts for short-term correlated fluctuations among $p_{\rm VV}(t)$, $V_{\rm VV}(t)$, and $T_{\rm VV}(t)$ with time.⁸¹ For example, the correlation coefficient $r(p_{\rm RV}, V_{\rm VV}) =$ -1.

Figure 14(a) shows $n_{\rm VV}(t)$ as function of time t for argon gas at $p_{\rm VV} = 857.4(7)$ Pa and $T_{\rm VV} = 296.78(4)$ K up to run time $t_{\rm run} = 876.325$ s. Here, the uncertainties of $p_{\rm VV}$ and $T_{\rm VV}$ are the combined type-A and -B uncertainties, dominated by the type-B uncertainty. The linear fit to the data is shown in Fig. 14(a) and determines \dot{n}_{VV} . The residuals $\delta n_{\rm VV}(t)$ of this fit are shown in panel (b) and are quite small. This impressive statistical sensitivity to $n_{\rm VV}$ results from using precise CDGs to measure pressure with short-term statistical uncertainty $u_A(p_{\rm RV})/p_{\rm RV} \sim 10^{-5}$, platinum resistance thermometers with short-term statistical uncer-

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FIG. 14. Measurement of flow out of the flowmeter $\dot{n}_{\rm FM} = 1.5598(17) \times 10^{-11}$ mol/s for argon at pressure $p_{\rm VV} = 857.4(7)$ Pa and $T_{\rm VV} = 296.78(4)$ K. (a) Molar number of argon atoms in the variable volume $n_{\rm VV}$ as a function of time. Blue points are experimental data, while the orange curve is the best linear fit to this data. (b) Residuals of the fit. (c) Binned residuals with a fit to a normal distribution (red curve). The standard deviation $\sigma = 1.1 \times 10^{-11}$ mol of the distribution corresponds to the statistical uncertainty in measuring $n_{\rm VV}(t)$. Reproduced from S. Eckel, D. S. Barker, J. Fedchak, E. Newsome, J. Scherschligt, and R. Vest, Metrologia **59**, 045014 (2022), public domain.

tainty $u_A(T_{\rm VV})/T_{\rm VV} \sim 10^{-6}$, and from precisely measuring small displacement rates of the piston. The residuals are to good approximation normally distributed with standard deviation $\sigma = 1.1 \times 10^{-11}$ mol as shown in Fig. 14(c). We cannot use naive linear least squares analysis to determine the type-A uncertainty $u_A(\dot{n}_{\rm VV})$ as there are correlations in the residuals. Thus, we repeat runs of the flowmeter, such as that shown in Fig. 14, multiple times and determine $\dot{n}_{\rm VV}$ and $u_A(\dot{n}_{\rm VV})$ by computing the mean and standard error in the mean of the fitted $\dot{n}_{\rm VV}$. Type-A uncertainties, calculated using six repeated runs, for three argon-gas flows $\dot{n}_{\rm FM}$, spanning two orders of magnitude, are summarized in Table II.

We now turn our attention to systematic (type-B) uncertainties, also summarized in Tab. II. Each of the quantities in Eq. (40)—pressure $p_{\rm VV}$, displacement volume $\Delta V_{\rm VV}$, temperature $T_{\rm VV}$, outgassing flow $\dot{n}_{\rm OG}$, and run time $t_{\rm run}$ —have an associated systematic uncertainty, the details of which can be found in Ref. 81. The uncertainties of these systematic, type-B contributions are uncorrelated. The contribution from the uncertainty in the pressure measurement $u(p_{\rm VV})$ dominates at all flows; itself dominated by the long-term stability of the bakeable CDGs described in Sec. III D 3. The uncertainty in the measurement of the total volume of the variable volume during the measurement $u(\Delta V_{\rm VV})$ is typically the next largest contributor, followed by the uncertainty in the temperature $u(T_{\rm VV})$. The uncertainty in the outgassing flow $u(\dot{n}_{\rm OG})$ is the second largest contributor at the lowest flows at around 10^{-13} mol/s, but is negligible for flows $\dot{n}_{\rm FM} > 10^{-12}$ mol/s. Finally, the contribution from the uncertainty in timing $u(t_{\rm run})$ is negligible. For all flows, the type-A uncertainty is at least twice as large as the type-B uncertainty after six averages of $t_{\rm max} \approx 850$ s runs.

The data in Table II differs from that in Ref. 81 in four ways. First, we only include flows in the range of interest for validation of the CAVS. Second, for this article we use the bakeable CDGs discussed in Sec. III D 3, which have a two to three times larger uncertainty than the transfer standards used in Ref. 81. Third, corrections from the non-ideality of the gas in the variable volume for flows less than 10^{-10} mol/s shown in the table are negligible. Finally, we omit contributions from linear drifts in $p_{\rm VV}$ and $T_{\rm VV}$; their relative contributions to $u(\dot{n}_{\rm FM})/\dot{n}_{\rm FM}$ are less than 3×10^{-4} as in Ref. 81.

For validation of the CAVS, we target pressures p_1 in the first chamber of the dynamic expansion system of 10^{-8} Pa to 10^{-6} Pa, as these pressures produce easily measurable sensor-atom loss rates between 0.01 s^{-1} and 1 s⁻¹. For N₂, the roughly 50 nL/s conductance of the fixed leak downstream of the variable volume, combined with the $C_0 = 37.22(3)$ L/s of the orifice connecting the two chambers of the dynamic expansion system, implies that our target pressure range requires us to fill the flowmeter to pressures between 10 Pa and 1 kPa, provided we do not use the optional flow splitter. Note that because both conductances scale in the same manner with mass, the fill pressure is gas-species independent. In this fill range, the flow meter produces N_2 flows between 2×10^{-13} mol/s and 2×10^{-11} mol/s with a relative uncertainty of about or better than 1 %, adding type A and B uncertainties, according to Table II. This combined uncertainty is larger than uncertainty of C_0 and the uncertainty in the measurement of the pressure ratio $r_{\rm p}$; thus it dominates the uncertainty p_1 .

6. Evacuation

The flowmeter must be evacuated of unwanted gases before initial use as well as before choosing to work with a different atomic or molecular gas. Our device can be evacuated through a rough pump or through a turbo pump connected to a large expansion volume as shown in the bottom right part of Fig. 6. We first pump down with the rough pump until the pressure at the rough pump, as read by a thermocouple gauge, is below 13 Pa while simultaneously ensuring that the pressure in the reference volume has dropped below 1000 Pa. We chose the 13 Pa pressure near the rough pump to guarantee that the flow is still laminar in the 4.45 mm diameter distribution tubings connecting the various volumes of the flowmeter and to prevent backflow of gas from the rough pump into the flowmeter. Flow in these tubings remains laminar down to a pressure of 0.13 Pa.

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			flow $\dot{n}_{\rm FM}$	
Source/Contribution	$2.35(1) \times 10^{-13} \text{ mol/s}$	$2.411(5) \times 10^{-12} \text{ mol/s}$	$ 1.524(3) \times 10^{-11} \text{ mol/s} $	
Pressure in variable volume	$u(p_{\rm VV})/p_{\rm VV}$	0.0032	0.0025	0.0022
Change in volume of variable volume	$u(\Delta V_{\rm VV})/\Delta V_{\rm VV}$	0.0007	0.0007	0.0007
Temperature of the flowmeter	$u(T_{\rm VV})/T_{\rm VV}$	0.0001	0.0001	0.0001
Outgassing of the variable volume	$u(\dot{n}_{ m OG})/\dot{n}_{ m FM}$	0.0009	9×10^{-5}	9×10^{-6}
Time measurement (computer clock)	$u(t_{ m run})/t_{ m run}$	2×10^{-6}	2×10^{-6}	2×10^{-6}
Total type-B	$u_B(\dot{n}_{ m FM})/\dot{n}_{ m FM}$	0.0034	0.0026	0.0023
Total type-A	$u_A(\dot{n}_{ m FM})/\dot{n}_{ m FM}$	0.012	0.005	0.004
Total	$u(\dot{n}_{ m FM})/\dot{n}_{ m FM}$	0.012	0.006	0.0046

TABLE II. One-standard-deviation uncertainty budget of the flowmeter's output $\dot{n}_{\rm FM}$ at three argon gas flows $\dot{n}_{\rm FM}$. Values are relative uncertainties contributing to $u(\dot{n}_{\rm FM})/\dot{n}_{\rm FM}$. The uncertainties in the first five rows are of type B and are added in quadrature, assuming that they are uncorrelated, to lead to the total type-B uncertainty. The sources of type-B uncertainties are explained in Ref. 81. The type-A uncertainty is determined from six experimental runs with $t_{\rm run} \approx 850$ s measuring $n_{\rm VV}(t)$. The total uncertainty is the uncorrelated combination of type-A and type-B uncertainties.

Once the pressure at the rough pump has been decreased to 13 Pa, the valve connecting the rough pump to the variable volumes, ballast volume, and reference volume is closed. The valves connecting the expansion volume and turbo pump to the flowmeter are opened and gas is pumped away with the turbo pump. When these valves actuate, however, a burst of gas is released into the expansion volume, which could potentially exceed the maximum pressure for safe operation of the turbo pump (about 100 Pa) if the expansion volume is too small. We empirically find that an expansion volume of 6 L is sufficient to limit the initial pressure increase to 5 Pa. The pressure in the expansion volume is read using a combination cold cathode/Pirani gauge.

The pressure in the expansion volume after the initial burst of gas is solely determined by the pressure in the various volumes multiplied by the ratio of the conductance of the distribution tubings to the pumping speed of the turbo pump. In our flowmeter this ratio is of order 10^{-3} . Our setup limits the maximum pressure at the turbo pump in steady state to about 1 Pa, well within acceptable limits of turbo pump operation. After some time, typically 12 h, the turbo pump decreases the pressure in all components of the flowmeter to base pressure, $< 10^{-5}$ Pa, determined by the balance between hydrogen outgassing from all surfaces and the pumping speed.

IV. LABORATORY-BASED CAVS

In combination with the flowmeter and dynamic expansion system of Sec. III, the laboratory-based coldatom vacuum standard has been designed to validate operation of the CAVS with the lowest possible uncertainties. In many respects, the CAVS resembles common laser-cooling apparatuses—utilizing magnetooptical traps (MOTs), magnetic traps, and radiofrequency (RF) antennas to hold and cool sensor atoms with a few unique features added for the purpose of measuring vacuum. Following a general introduction, the subsequent subsections describe these unique features. For a detailed overview of laser cooling physics, MOTs, and magnetic traps, we refer the interested reader to the vast literature on these topics, ^{35,86–89} or to our prior primers on laser cooling in the context of vacuum metrology.^{90,91}

Figure 15 shows a computer-assisted design (CAD) model of the laboratory-based CAVS. It is divided into two chambers: a cold-atom source chamber with large pumps and a vacuum measurement chamber connected to the dynamic expansion system, separated by a 1.80(2) mm diameter, 18.09(3) mm long differential pumping tube. The conductance of the tube is 0.033 Ls^{-1} for N₂ and 0.12 Ls^{-1} for H₂ at T = 295 Kbased on Eqs. (33) and (34). This conductance must be small compared to the conductance C_0 of the orifice connecting the two chambers of the dynamic expansion system, in order to minimize flow from the flowmeter into the region of the cold-atom source where the gas would be pumped away. Corrections to the pressure in the first chamber of the dynamic expansion system p_1 due to this small differential pumping tube will be on the order of the ratio of the conductances, $< 10^{-4}$.

The cold-atom source uses an alkali metal dispenser that effuses atoms which are subsequently cooled and formed into a cold atomic beam traveling along the y axis by a two-dimensional magneto-optical trap (2D MOT). The atom source produces either cold rubidium or lithium atoms. As described in Sec. IV A, this 2D MOT has the unique feature that it uses tilted effusive sources to eliminate the push-beam found in other 2D MOT setups.

The pressure in the cold-atom source's chamber never rises above 10^{-7} Pa during normal operation and represents a minimal gas load on the dynamic expansion system. This 10^{-7} Pa is impressive, given that rubidium has a high vapor pressure of 2×10^{-5} Pa at room temperature. An aluminum cold shroud envelopes the 2D MOT to capture all atoms emitted by the effusive sources not captured by the 2D MOT. The shroud is cooled via two externally mounted thermo-electric chiller (TEC) assemblies, each containing two 26 W TECs, themselves water



FIG. 15. The cold-atom source chamber, with its pumps and cold shroud, and the vacuum measurement chamber, encased in Bitter coils, are located on the left and right hand side of the drawing, respectively. The two chambers are only connected by a differential pumping tube. The connection to the dynamic expansion system is located on the far right hand side of the CAVS. The 2D MOT magnetic field is generated by a combination of permanent magnets (red and blue rectangles, where red and blue indicate the opposite poles) and circular copper coils. A full description can be found in the text. Note the coordinate system in the bottom right hand corner with the z axis anti-parallel to earth's gravitational acceleration. Red arrows denote laser beams for the 2D and 3D magneto-optical traps. The device along the y axis is 0.76 m long. Abbreviations used: NEG: non-evaporable getter pump; AMD: alkali metal dispenser; and TEC Assy: thermo-electric cooler assembly.

cooled and connected to the shroud via two 6.35 mm diameter copper feedthroughs. The TECs maintain the shroud at -30 °C. This temperature is low enough to keep the vapor pressure of rubidium $\lesssim 3 \times 10^{-7}$ Pa and likewise that of lithium $\lesssim 10^{-17}$ Pa. Other gases, *e.g.* water, nitrogen, and hydrogen, in the cold-atom source chamber are pumped away by a 400 L/s non-evaporable getter pump for H₂ and a 60 L/s ionization pump.

In the vacuum measurement chamber, atoms from the 2D MOT are captured, further cooled, and trapped in a 3D MOT and then subsequently transferred into either a quadrupole or Ioffe-Pritchard magnetic trap. This chamber is a 3.8 cm \times 2.9 cm \times 10.2 cm borosilicate glass cell. On one end, it attaches to the differential pumping tube; on the other, to the dynamic expansion system of Sec. III B. The chamber is surrounded by a Bitterstyle^{92–94} electromagnet capable of generating both types of magnetic traps. The Bitter coil electromagnet is described in detail in Sec. IV B and Ref. 95. Vertical MOT beams enter through the central holes in the Bitter coils. Optical access in the horizontal plane allows for radial MOT beams to enter the chamber. A CCD camera mounted along the x axis captures both fluorescence and

absorption images of the atoms.

The temperature of the glass cell and thus of gas in the chamber is monitored by four platinum resistance thermometers (PRTs) mounted on opposite corners. Two sets of two square RF loop antennas, located outside of the glass cell and between the Bitter coil assemblies and not shown in Fig. 15, create oscillating magnetic fields in the xy plane that act as an RF knife to remove high kinetic energy atoms from the cloud. The presence of Bitter coils strongly attenuate RF fields in the \hat{z} direction. The frequencies of the RF fields set the depth of the magnetic trap for the cold atoms. Their amplitude is at most 150 mT, corresponding to maximum resonant Rabi frequency of about 50 kHz for the $|F, M\rangle = |1, -1\rangle$ to $|1, 0\rangle$ hyperfine transition of the electronic ground state of ⁷Li and ⁸⁷Rb.

As of this writing, we have trapped 85 Rb, 87 Rb, and ⁷Li in 3D MOTs in the CAVS measurement chamber. We have magnetically trapped 87 Rb and have made preliminary comparisons of the 87 Rb loss rate coefficients with those from theory. The operation of these experiments and preliminary measurements are described in Sec. IV C.

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A. The cold atomic source: a push-beam free 2D MOT

Cold-atom sources based on two-dimensional MOTs are quite common. They can be loaded either from a background gas or from an effusive atom dispenser like an oven with an output aperture hole. Often, these effusive dispensers are placed in the 2D plane spanned by the 2D MOT beams. An additional "push" beam in the remaining perpendicular direction, co-linear with the axis of the 2D MOT, pushes the captured atoms to form a cold atomic beam. This design has been very successful: the resulting cold atomic beam can be both very bright and captured by a 3D MOT downstream. Unfortunately, the push beam often acts as an undesired perturbation on this downstream 3D MOT. The authors of Refs. 96 and 97 suggested that mounting an effusive source out of the 2D plane spanned by the MOT beams makes a "push" beam unnecessary. After the atomic velocity components in the plane of the 2D MOT beams are cooled, the residual forward velocity of the atoms makes a slow atomic beam.

Our Li and Rb cold-atom source creates such beams with push-beam-free 2D MOTs. The 2D MOT beams are directed along the four directions $(\pm 1, 0, 0)$ and $(0, 0, \pm 1)$ in the xz plane using the coordinate system defined in Fig. 15. The 2D quadrupole field $\mathbf{B}(x, y, z)$ for this MOT is generated by a combination of permanent- and electromagnets. Near the axial center of the 2D MOT, the magnetic field is independent of y and the constant derivatives satisfy $dB_z/dz = -dB_x/dx$ and $\mathbf{B}(x = 0, y, z =$ 0) = 0, for all y. For ⁷Li, $dB_x/dx \approx 5.0$ mT/cm; for ⁸⁷Rb, $dB_x/dx \approx 1.2 \text{ mT/cm}$.

Our 2D MOTs are loaded by alkali metal dispensers, one for Li and one for Rb, permanently connected to the source chamber. The lithium and rubidium dispensers point to the center of the 2D MOT and preferentially emit atoms along $(-\sin\theta_{2\rm D}/\sqrt{2},\cos\theta_{2\rm D},\sin\theta_{2\rm D}/\sqrt{2})$ and $(\sin\theta_{2\rm D}/\sqrt{2},\cos\theta_{2\rm D},\sin\theta_{2\rm D}/\sqrt{2})$, respectively, where $\theta_{2\rm D}$ is the angle between the emission vector and y axis, that is the axis of our 2D MOT. For $\theta_{2D} = 90^{\circ}$ the dispensers lie in the xz plane. The optimal value for angle θ_{2D} needed to be determined during the design phase, as our apparatus has too many other constraints to allow for changing the orientation of the effusive sources after assembly.

We use a geometric model, shown in the inset of Fig. 16, to determine the optimal value for angle θ_{2D} . An effusive dispenser at a distance $L_{\rm S}$ from the center of the 2D MOT emits atoms into its capture region. The flux of Li or Rb atoms with velocities between v and v + dvemitted from infinitesimal area dA_S within the output aperture of the dispenser into solid angle $d\Omega$ around angle θ with respect to the primary axis of the dispenser is⁹⁸

$$I(v,\theta) \, d\Omega \, \mathrm{d}v \, \mathrm{d}A_{\mathrm{S}} = \rho_{\mathrm{S}}[v\cos\theta] f(v) \, d\Omega \, \mathrm{d}v \, \mathrm{d}A_{\mathrm{S}} \,, \quad (61)$$

where $\rho_{\rm S}$ is the number density of the gaseous alkali-metal atoms in the dispenser and f(v)



Computed ⁷Li number distributions $N_{2D}(v_y)$ as FIG. 16. functions of the velocity v_{y} along the axis of the CAVS 2D MOT sourced from a tilted, effusive sensor-atom dispenser at four angles θ_{2D} relative to the negative y axis defined in Fig. 15. The dispenser has area opening $A_{\rm S} = 0.3 \text{ cm}^2$ and is at temperature $T_{\rm S} = 350$ °C, corresponding to an atom number density $\rho_{\rm S} \approx 10^{11} {\rm ~cm^{-3}}$ inside the dispenser. Vertical black lines show the minimum and maximum velocities that can be captured by the 3D MOT in the measurement chamber of the CAVS. The inset shows the location and orientation of the effusive dispenser (tilted rectangle) relative to the center of the 2D MOT. The dashed horizontal line is the positive yaxis of the 2D MOT. The circle of radius $r_{\rm B}$ represents the spatial capture region of the 2D MOT. Cooled sensor atoms move to the right parallel to the axis of the 2D MOT. The dispenser is placed a distance $L_{\rm S}$ away from the center of the 2D MOT.

 $4\pi v^2 \exp[-mv^2/(2kT_{\rm S})] \times (m/(2\pi kT_{\rm S}))^{3/2}$ is the probability distribution of velocity v of atoms with mass m at temperature $T_{\rm S}$ inside the dispenser with $\int_0^\infty f(v) dv = 1$

Atoms that enter the capture volume – the spatial region where all four laser beams overlap – and have a velocity that is less than capture velocity v_c of the 2D MOT have their velocity in the plane of the 2D MOT beams cooled to near zero, while their forward velocity v_{μ} is unaffected. Atoms that do not satisfy these two criteria do not contribute to the flux of the cold-atom source. To calculate this flux of cold atoms, we apply three simplifying assumptions. First, we approximate the capture volume by a sphere of radius $r_{\rm B}$. We have $r_{\rm B} \approx 1.4$ cm corresponding to the measured apertured beam radii of our four laser beams. Second, we assume that the area of the output aperture of the dispenser, $A_{\rm S}$, is small compared to the size of the atom cloud in the 2D MOT so that the integrand $I(v, \theta)$ in Eq. (61) is independent of $A_{\rm S}$. Third, we assume a spatially-independent capture velocity v_c for the 2D MOT given by the maximum velocity for which the atoms can be decelerated to a stop

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given the maximum force the laser beams exert. We have

$$v_{\rm c} = \sqrt{\hbar k_{\rm L} \Gamma_i r_{\rm B}/m} \,, \tag{62}$$

where $k_{\rm L}$ is the wavevector of the lasers, $\Gamma_{i={\rm Li,Rb}}$ are the natural decay rates of the electronically excited state used for laser cooling, $1{\rm s}^22{\rm p}({}^2{\rm P}_{3/2})$ of ⁷Li and [Kr]5p(${}^2{\rm P}_{3/2}$) of ⁸⁷Rb, respectively. Note that $\hbar k_{\rm L}\Gamma_i/(2m)$ is the maximum acceleration or deceleration that can be created with Doppler cooling.⁸⁸ Differences in wavelengths of the four laser beams are negligible for our approximate analysis. For our parameters, $v_c \approx 240$ m/s for ⁷Li and $v_c \approx 60$ m/s for ⁸⁷Rb. The maximum deceleration, however, is rarely achieved because of both limited laser power and competition of scattering from both coand counter-propagating beams. Hence, we reasonably use $v_c \approx 120$ m/s for ⁷Li and $v_c \approx 30$ m/s for ⁸⁷Rb, *i.e.* half the values, for the subsequent calculation.

After some thought and accounting for the threedimensional geometry of the effusive dispenser, the flux density of atoms emitted from the source $N_{2D}(v_y)$ at velocity v_y along the 2D MOT axis is then given by

$$N_{2\mathrm{D}}(v_y;\theta_{2\mathrm{D}}) = A_{\mathrm{S}} \int_0^{\theta_0} \sin\theta \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \int_0^{v_c} \mathrm{d}v I(v,\theta)(63) \\ \times \delta(v_y - v[-\sin\theta_{2\mathrm{D}}\sin\theta\cos\phi + \cos\theta_{2\mathrm{D}}\cos\theta]),$$

with $\tan \theta_0 = r_{\rm B}/L_{\rm S}$ and $\delta(x)$ is the one-dimensional delta function. We numerically integrate Eq. (63).

The results of calculations for ⁷Li are shown in Fig. 16 for four $\theta_{\rm 2D}$ and L_S = 45 mm, A_S = 0.3 cm², and T_S = 350 °C, corresponding to a number density $\rho_S \approx$ 10^{11} cm⁻³ inside the dispenser. Figure 16 also shows the slowest and fastest ⁷Li beam velocities that we believe can be captured by the 3D MOT in the measurement chamber. The lower limit of 10 m/s corresponds to the velocity with which an atom can leave the 2D MOT and clear the differential pumping tube between the source and measurement chamber if its transverse velocity corresponds to the average velocity of a ⁷Li atom at the Doppler temperature $T_{\rm D} = \hbar \Gamma_{\rm Li}/2$. The upper limit of 60 m/s corresponds to our estimate of the capture velocity of the 3D MOT. From Fig. 16, we realize that $\theta_{2D} = 60^{\circ}$ is optimal as most of the flux density $N_{2D}(v_{u};\theta_{2D})$ falls within the 10 m/s and 60 m/s window. This optimum angle is roughly the same for ⁸⁷Rb and ⁷Li.

Finally, the derivation of Eq. (63) neglects momentum diffusion during the capture process into the 2D MOT. Diffusion would further broaden the 2D MOT output beam's velocity distribution by $\sqrt{v_c v_R}$, where $v_R = \hbar k_L/m$ is the atomic recoil velocity. The scaling can be understood through photon counting: fully decelerating atoms from a velocity v_c requires a minimum of $N_{\rm ph} = v_c/v_R$ photons, and the additional random velocity broadening from scattering this many photons is $v_R \sqrt{N_{\rm ph}}$. For ⁷Li, which has $v_R = 8.5$ cm/s, the additional broadening is on the order of 4 m/s, which is small compared to the widths of the features shown in Fig. 16. The atomic sources are commercially-available alkalimetal dispensers. Each dispenser contains approximately 1 g of solid alkali metal. The lithium source is loaded with pure, natural-abundance lithium pellets; the rubidium source is loaded with a natural abundance rubidiumbismuth eutectic. Our lithium dispenser require approximately 30 W of power to vaporize solid lithium; whereas the rubidium dispenser requires about 3 W. They are mounted on top of two copper rods, and are pointed toward the center of the 2D MOT.

The optimal quadrupole magnetic fields for the 2D MOT are different for lithium and rubidium. A combination of permanent magnets and electromagnets allows switching between the two required field gradients, while dissipating the least amount of power. Eight neodymium-iron magnets, each 9 mm thick by 10 mm wide by 25 mm long with residual magnetization of 1.275 A/m, are mounted to the outside of the source chamber along the tubes that the 2D MOT laser beams travel through. Four of these magnets are visible in Fig. 15. The permanent magnets produce a magnetic field with gradients $dB_x/dx = -dB_z/dz = 3 \text{ mT/cm}$ near the center of the source chamber. In addition, each tube holds a pair of water-cooled copper coils connected in series. Their design is based on those in Ref. 99; each coil is made from ≈ 50 turns of 0.33 mm thick, 6.35 mm wide Kapton-coated copper ribbon. The coils are held together with thermally-conductive epoxy, attached to aluminum mounts, and pressed against a copper tube carrying cooling water. The four electromagnets (each comprised of a single pair of coils) are controlled independently of each other by bipolar, current supplies capable of delivering up to ± 20 A.¹⁰⁰

The electromagnets strengthen or weaken the quadrupole field generated by the permanent magnets depending on the direction of the current in the coils. When running +20 A of current through each coil the quadrupole magnetic field gradient changes to $dB_x/dx = 6 \text{ mT/cm}$; when running -20 A, the coils change dB_x/dx to 0 mT/cm. A current magnitude of 20 A dissipates 60 W of heat in each of the eight electromagnets. The operating field gradient of the 2D MOT is $dB_x/dx = 5 \text{ mT/cm}$ for lithium and 1.2 mT/cm for rubidium. Because each coil pair has its own current supply, they also can shift the position of magnetic field zero of the 2D MOT, helping to align the 2D MOT with respect to the narrow differential pumping tube.

For both lithium and rubidium operation, the 2D MOT cooling light is nearly resonant on the so-called D_2 transition between their ${}^2S_{1/2}$ ground and first ${}^2P_{3/2}$ excited electronic states. In fact, the 2D MOT cooling light is detuned by $\Delta_{2D} = -2\pi \times (9 \text{ MHz})$ from the hyperfine-resolved ${}^2S_{1/2} (F = 2) \rightarrow {}^2P_{3/2} (F' = 3)$ optical cycling transition, where F and F' are the total angular momentum quantum number of the ground and excited state, respectively. Here, $\hbar\Delta$ has units of energy. The natural decay rates of the ${}^2P_{3/2}$ state in lithium and rubidium are $\Gamma_{\text{Li}} \approx 2\pi \times 5.87$ MHz and $\Gamma_{\text{Rb}} \approx 2\pi \times 6.07$ MHz,

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This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0120500 respectively, so $\Delta_{2D}/\Gamma_{\text{Li, Rb}} \approx -1.5$ for both elements. (To very good approximation these decay rates are independent of hyperfine state F' of the ${}^{2}\text{P}_{3/2}$ electronic state.)

Laser light for ⁷Li is generated by a solid-state pumped Ti:Sapphire laser. Laser light for ⁸⁷Rb is generated by an external cavity diode laser with a tapered amplifier. The laser beams for the lithium- and rubidium-based CAVSs use the same mirrors and other optics to guide them through the vacuum chamber. The vertical and horizontal laser beams for the 2D MOT in Fig. 15 are retroreflected and each contain approximately 125 mW and 50 mW of power for lithium and rubidium, respectively. The beams are circularly polarized with vertical and horizontal laser beams having opposite circular polarization.

Atoms that are off-resonantly scattered into the ${}^{2}\mathrm{S}_{1/2} \left(F=1\right)$ state must be returned to the ${}^{2}\mathrm{S}_{1/2} \left(F=2\right)$ state via resonant optical pumping on the ${}^{2}S_{1/2}(F)$ 1) $\rightarrow {}^{2}P_{3/2}(F'=2)$ "repump" transition. For lithium, an electro-optic modulator (EOM) frequency modulates the 2D MOT beams at approximately $2\pi \times (813 \text{ MHz})$, so that the $+1^{st}$ -order sideband is detuned by Δ_{2D} from the lithium repump transition. The power of the RF drive for the EOM is set to produce a cooling to repump power ratio of two to one. At this drive, the amount of optical power in the carrier, which corresponds to the cooling light, is reduced to 50 % of the total power. The power in the repump sideband is then 25 % of the total optical power; another 25 % of the total optical power is in a fardetuned sideband and is not used. The cooling power Pin the lithium 2D MOT beams is therefore approximately 63 mW.

For rubidium, the repump light is generated by a distributed-Bragg reflector laser and is made to have the same spatial profile as that of the cooling light by combining their light with a single-mode, polarization-maintaining fiber-optic beam splitter. The cooling power in the rubidium 2D MOT beams remains P = 50 mW, the laser power in the repump beams is approximately 4 mW.

The 2D MOT beam profiles are to good approximation Gaussian for both lithium and rubidium cooling and repump light. All beams have the same beam waist w of 1.4 cm, the distance from the beam axis where the optical intensity drops to $1/e^2$ of the value on the beam axis. Hence, with peak cooling intensity at the focal point of the laser beams given by $I = 2P/(\pi w^2)$, the peak cooling saturation parameter $s^{\text{Li}} = I/I_{\text{sat}}^{\text{Li}} \approx 8$ for lithium and $s^{\text{Rb}} = I/I_{\text{sat}}^{\text{Rb}} \approx 10$ for rubidium, where $I_{\text{sat}}^a = (\hbar \omega_a)^3 \Gamma_a/(12\pi \hbar^2 c^2)$ is the saturation intensity for the $^2\text{S}_{1/2}(F = 2, M = \pm 2) \rightarrow ^2\text{P}_{3/2}(F' = 3, M' = \pm 3)$ transition of atom $a = ^7\text{Li}$ or ^{87}Rb driven by the appropriate circularly-polarized light. The energies $\hbar \omega_a$ are the electronic transition energies with respect to the barycenters of the hyperfine splittings in the ground and excited states. The saturation intensities are $I_{\text{sat}}^{\text{Li}} \approx 2.54 \text{ mW cm}^{-2}$ and $I_{\text{sat}}^{\text{Rb}} \approx 1.67 \text{ mW cm}^{-2}$. (The sat-

uration intensity of the F = 1 to F' = 2 D_2 repump transition is the same as that of the cooling transition.)

B. Bitter coils

The Bitter coil electromagnets surrounding the measurement chamber have three primary design constraints. First, the electromagnets must be capable of generating the magnetic field configurations for both a quadrupole and a Ioffe-Pritchard (IP) trap. A quadrupole field is required for the 3D MOT, but is also a robust trap for vacuum sensing in the UHV range. The more complicated IP trap has a non-zero magnetic bias field B_0 at its center, which suppresses Majorana spin-flip losses (see Sec. IIA) to allow measurement of XHV vacuum pressures. Second, the electromagnets must preserve the high optical access of the glass cell. Third, the electromagnets must have very low thermal resistance. When measuring the atom loss rate at pressures below 10^{-7} Pa, the time that the atoms spend in the magnetic trap is much larger than that of preparing and measuring the atomic ensemble. We therefore require electromagnets that can operate close to our 100% duty cycle without overheating or deforming the magnetic trap.

The coil layout that satisfies the first two design considerations for the CAVS electromagnet is the cloverleaf design. This design uses three pairs of symmetrically mounted coils,^{31,32,34} one above and one below the glass measurement chamber, to create the magnetic field profile of a Ioffe-Pritchard trap

$$\mathbf{B}_{\rm IP}(\mathbf{x}) = B_0 \begin{pmatrix} 0\\0\\1 \end{pmatrix} + B' \begin{pmatrix} -y\\x\\0 \end{pmatrix} + \frac{B''}{2} \begin{pmatrix} -xz\\-yz\\z^2 - \frac{1}{2}(x^2 + y^2) \end{pmatrix}$$
(64)

in the coordinate system defined in the lower right hand corner of Fig. 15.¹⁰¹ The field of Eq. (64) has a non-zero magnetic field strength minimum at position $\mathbf{x} = \mathbf{x}_0 =$ $(0, 0, 0)^T$ inside the measurement chamber. The first pair of coils creates the "curvature" field proportional to B''and contributes to bias field B_0 . A pair of Helmholtz coils, called "anti-bias" coils, creates a uniform field that opposes, but does not fully cancel, the bias-field contribution from the curvature coils. Finally, a pair of "clover" coils creates the quadrupole gradient field proportional to B'. In each coil pair, the current in each of its coils has the same value and sense of circulation. The currents in different coil pairs are set independently, allowing independent control of B_0 , B', and B''.

The cloverleaf coil design can also produce a quadrupole magnetic field $\mathbf{B}_{quad}(\mathbf{x}) = B'_{quad}(-x/2, -y/2, z)^T$ for magnetic trapping or MOT operation. In the CAVS, we create the quadrupole field by switching the direction of current in one of the curvature coils while keeping the current to the clover and anti-bias coils turned off.

We built CAVS cloverleaf-style Ioffe-Pritchard traps

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FIG. 17. (Main image on the right) Rendering of one of the two CAVS Bitter coil assemblies for the cloverleaf trap. The Garolite G-10 water distribution manifold is white; a section has been cut away to show the geometries of the supply and collection reservoirs. Four leafs of the clover coil sit directly on the distribution manifold; one is hidden to allow viewing of the manifold interior. The anti-bias coils and the curvature coils are stacked on the clover coil, with an insulating G-10 spacer in between. (Left image) An exploded view of the clover coil and the anti-bias coil near their G-10 spacer (green). The curvature coil has been omitted for clarity. Insulating Teflon spacers (white) create channels for the flow of water between copper (dark, redish brown) and brass (yellowish brown) conductive coil layers. Pink arrows indicate the flow of electric current, while blue arrows indicate the flow of cooling water. Reproduced from J. L. Siegel, D. S. Barker, J. A. Fedchak, J. Scherschligt, and S. Eckel, Rev. Sci. Instrum. **92**, 033201 (2021), public domain.

using a stacked Bitter-type electromagnet. Figure 17 shows one of our two identical Bitter coil assemblies. The designs are adapted from those by Refs. 92–94 to allow for efficient cooling of the current-carrying copper and brass parts with deionized water and enable continuous operation. The assemblies have many parallel, high-wetted-area water-cooling channels to minimize hydraulic resistance and maximize heat transfer.¹⁰² Among recently published electromagnet designs for laser cooling applications, Bitter-type electromagnets offer the lowest thermal resistance.^{92–94,103–105} The assemblies satisfy our third design constraint and are described in detail in Ref. 95.

Each Bitter coil is composed of a stack of alternating conducting copper and insulating Teflon crescents mounted to a water-distribution manifold. The top conducting layers of all coils and the bottom conducting layer of the clover leaf coils are made of brass for structural support. The image on the left-hand side of Fig. 17 shows the current and water flows in the Bitter coil. The clover coils require radial cooling water flows, while the circular anti-bias and curvature coils require azimuthal water flows. All coil components have holes that align to form vertical cooling water columns that serve to supply and collect water from the Bitter coil stack. Cutouts in the insulating layers allow water to flow horizontally between neighboring supply and collection columns. The original water distribution manifold was 3D printed, but recently we switched to a Garolite G-10 subtractively-manufactured manifold.

We have measured the magnetic field profile generated by each of the three coil pairs separately. Measurements on the curvature coil pair have been conducted both with and without the direction of the current in one of its coils reversed, corresponding to the quadrupole and Ioffe-Pritchard configuration, respectively. Measurements using a three-axis Hall probe, a Lakeshore Model F71, were taken at a current of I = 100.00(5) A through one pair of coils at a time. The Hall probe was mounted to a three axis translation stage in order to map the magnetic field as a function of 3D position. We rely on the linearity of Maxwell's equations to extrapolate the field to other currents. This linearity should be accurate to better than 1 part in 10^4 given that the Bitter coil contains no magnetically non-linear (ferrous) materials.

The center \mathbf{x}_0 of the anti-bias and curvature coil pairs correspond to saddle points in $|B_z|$ in the Ioffe-Pritchard configuration. Hence, our experimental procedure is to first find \mathbf{x}_0 with the Hall probe. We then verify our alignment with the z axis, defined in Fig. 15, by moving the probe along z and ensuring that $B_x = B_y = 0$. Consequently, B' = 0 in Eq. (64). We then record B_z at x = y = 0 along z at approximately 10 points and fit these data to $B_z = B_0 + B'' z^2/2$, where z is measured relative to \mathbf{x}_0 . We find that the centers of the anti-bias and curvature coils are within 0.5 mm of each other suffi-

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	Anti-bias	Curvature	Clover			
	coil pair	coil pair	coil pair			
Ioffe-Pritchard magnetic trap						
$B_0/I ~(\mu T/A)$	154.75(8)	-151.3(2)	-6.613(4)			
$B'/I \ (\mu T/(cm A))$	—	—	36.9(1)			
$B''/I \ (\mu T/(cm^2 A))$	-2.82(2)	-50(2)	0.62(3)			
Quadrupole magnetic trap						
$B'_{\rm quad}/I~(\mu T/({\rm cm A}))$		82.9(2)				
Single-coil electrical parameters						
Inductance (μH)	21(1)	5.0(4)	68(5)			
Resistance $(m\Omega)$	9.2(6)	13.0(9)	32(2)			

TABLE III. Measured magnetic field and electrical parameters for the anti-bias, curvature, and clover coil pairs of the CAVS electromagnets arranged to generate an Ioffe-Pritchard or a quadrupole trap. The parameters measured in the Ioffe-Pritchard configuration are the magnetic field strength per unit current B_0/I , gradient per unit current B'/I, curvature per unit current B''/I, coil pair inductance and coil pair resistance. The gradient per unit current B'_{quad}/I in the quadrupole configuration needed only to be measured for the curvature coil pair. Dashes indicate field parameters that are strictly zero by symmetry. The resistance and inductance of a single coil in a pair are taken from Ref. 95. Differences in resistance and inductance between the coils in a pair are unimportant for operation of the trap.

ciently close for reliable operation of the atomic traps.¹⁰⁶

To determine B'_{quad} for the curvature pair in the quadrupole configuration, when the current in one of the coils is reversed, we first find the position where the magnetic field strength is zero. This determines the geometric center of the coil pair; the z axis is the same as for our measurements with the curvature coil pair in the IP configuration. We then record B_z at x = y = 0 along z at approximately 10 points and fit these data to $B_z = B'_{quad}z$. For the curvature coil pair, we find that the position of the field zero in the quadrupole configuration and the position of the field saddle point in the IP configuration are the same to within 0.5 mm.

Finally, we reposition the translation stage to measure B' for the clover coil pair. For this coil, we work in a rotated x'-y' plane that is rotated by $+45^{\circ}$ about the z axis. The translation stage moves the Hall probe along the x' axis. We first find the position $\mathbf{x} = \mathbf{x}' = (0, 0, 0)^T$. At this position, B_z is maximal along the z direction and, simultaneously, $B_{x'} = 0$ and $B_{y'} = 0$. We verify alignment with the x' axis by ensuring that $B_{y'} = 0$ for all x' with (y', z) = (0, 0). Then at (y', z) = (0, 0), we record $B_{x'}$ along the x' axis at approximately 10 points and fit these data to $B_{x'} = B'x'$. We further record B_z at (x', y') = (0, 0) [or (x, y) = (0, 0)] along z and fit the results to $B_z = B_0 + B'' z^2/2$. Because the translation stage was repositioned, we cannot determine the center of the clover coil pair relative to the other two coil pairs, but we believe it to be displaced by less than 0.5 mm.

Table III lists the relevant fitted magnetic field coefficients B_0 , B', and B'' divided by the applied current as well as their uncertainties. For each entry, we add the



FIG. 18. Measurement of the inductance $L_{\rm B}$ and resistance $R_{\rm B}$ of an individual clover coil. The blue curve with left y axis corresponds to the measured voltage across the coil $V_{\rm out}$ in response to a triangular current drive I, shown as the red curve with right y axis. Both curves are shown as a function of time t. The voltage response is fit to the sum of a triangle and a square wave in order to extract $L_{\rm B}$ and $R_{\rm B}$ (see text), shown as the dashed black curve. Figure adapted from J. L. Siegel, D. S. Barker, J. A. Fedchak, J. Scherschligt, and S. Eckel, Rev. Sci. Instrum. **92**, 033201 (2021), public domain.

relative uncertainties in the fitted magnetic field coefficients and the current in quadrature assuming no correlations. The clover coil pair contributes a small but non-negligible amount to the IP trap B_0 and curvature B'' due to a quirk of the Bitter coil layout. We also calculated the field strengths using Radia.¹⁰⁷ The calculations and measurements agree to better than 3% for the curvature and anti-bias coils and to 10% for the more complicated clover coil.

In operation, the current flowing in the Bitter coil changes with time. For example, when changing from a magneto-optical trap to a magnetic trap, the current is rapidly increased to transfer atoms effectively. Likewise, when counting the number of atoms with absorption imaging, the magnetic trap must be turned off rapidly to avoid adverse atomic Zeeman shifts. To find the characteristic current switching time, we measure the inductance and resistance of an individual coil in a pair by modulating the current through the coil with a 100 Hz triangle wave. Figure 18 shows the measured voltage across the coil and applied current as functions of time for a clover coil. The electrical circuit for this measurement is a resistor with resistance $R_{\rm B}$ in series with an inductor with inductance $L_{\rm B}$ driven by a current source with a periodic time-dependent current I(t). The voltage response, the sum of that of the resistor and inductor, $V_{\text{out}}(t) = I(t)R_{\text{B}} + L_{\text{B}}dI(t)/dt$ is then the sum of a triangle wave and its derivative, a square wave. The amplitude of the triangle wave in the voltage response yields the resistance and the amplitude of the square wave yields the inductance. Figure 18 also shows an example fit; the fitted $R_{\rm B}$ and $L_{\rm B}$ of the three coils are presented in Table III. The characteristic current switching times $L_{\rm B}/R_{\rm B}$ for the curvature, anti-bias, and clover coils are 0.05 ms, 0.3 ms, and 2 ms, respectively.

The Bitter coil electromagnets are water cooled with a

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manifold that allows a maximum flow of 10.0(3) L/min at a differential pressure of 190(10) kPa. The thermal resistance of the anti-bias and clover coils at the maximum water flow are 4.2(1) °C/kW and 2.5(1) °C/kW, respectively, as measured with *in-situ* thermocouples. The thermal resistance of the curvature coil is measured using a thermal imaging camera, as the geometry of the CAVS apparatus prevents us from installing a thermocouple on the curvature coils. Their thermal resistance lies between that of the clover and anti-bias coils. At the nominal operating current of 200 A, the maximum temperature rise between any point on the Bitter coil assembly and the temperature of the cooling water is 5.8 °C, which is achieved in less than 10 min after the current is turned on. The maximum temperature difference between any two points on the anti-bias and clover coil pairs at the nominal operating current is approximately 2.7 °C. The low thermal resistance of the CAVS electromagnets allows continuous operation up to the maximum output of our power supplies.

C. Three-dimensional magneto-optical traps for the CAVS

Atoms from the 2D MOT enter the measurement chamber through the differential pumping tube and are loaded into a 3D MOT. As in the 2D MOT, the ⁷Li and 3D MOT cooling and repump lasers operate on the hyperfine-resolved D_2 transitions $2^2 S_{1/2} (F=2) \rightarrow$ $2^2 P_{3/2} (F' = 3)$ and $2^2 S_{1/2} (F = 1) \rightarrow 2^2 P_{3/2} (F' = 2)$, respectively. In the 3D MOT, both lasers are detuned by $\Delta/\Gamma_{\rm Li} = -5$, where again $\Gamma_{\rm Li}$ is the natural decay rate of the $1s^2 2p(^2P_{3/2})$ excited state of ⁷Li. The laser light comes from the same Ti:Sapphire laser that creates the light for the 2D MOT. The 2D and 3D MOTs also share the same 813 MHz EOM for generating the repump light. The ratio between the optical power addressing the cooling transition to the total optical power is 50 %, that for the repump laser is 25 %, identical to those for the 2D MOT. The ⁷Li 3D MOT uses a quadrupole magnetic field with a gradient of $B'_{\text{quad}} = 2.5 \text{ mT/cm}$, generated by the curvature coil pair discussed in the last subsection.

The ⁸⁷Rb 3D MOT also shares its laser sources with the 2D MOT, but uses slightly different detunings. The frequency of the cooling laser is detuned by $\Delta/\Gamma_{\rm Rb} =$ -3.5 from the $5^2 S_{1/2} (F = 2) \rightarrow 5^2 P_{3/2} (F' = 3)$ transition, while the frequency of the repump light is detuned by $\Delta/\Gamma_{\rm Rb} = +1.0$ from the $5^2 S_{1/2} (F = 1) \rightarrow$ $5^2 P_{3/2} (F' = 2)$ transition. The ⁸⁷Rb 3D MOT uses a quadrupole magnetic field with a field gradient of $B'_{\rm quad} = 2.2 \text{ mT/cm}.$

The six Gaussian-shaped cooling and repump laser beams for both 3D MOTs have a $1/e^2$ radius of approximately 1.1 cm. For ⁷Li, the 20 mW of laser light per beam leads to a saturation parameter $s_{\rm cool} = I_{\rm cool}/I_{\rm sat}^{\rm Li} \approx 4$ on the cooling transition, where I is the peak laser intensity and $I_{\rm sat}^{\rm Li}$ is the again saturation intensity for the ${}^2{\rm S}_{1/2}(F = 2, M = \pm 2) \rightarrow {}^2{\rm P}_{3/2}(F' = 3, M' = \pm 3)$ transition of ⁷Li. Likewise, the 10 mW repump beams each have a saturation parameter of $s_{\rm repump} \approx 2$. For ⁸⁷Rb, 27 mW cooling beams each have a saturation parameter $s_{\rm cool} = I_{\rm cool}/I_{\rm sat}^{\rm Rb} \approx 8.5$; the 250 μ W repump beams have $s_{\rm repump} \approx 0.1$.

The 3D MOT cools the sensor atoms to temperatures on the order of 1 mK for ⁷Li and 100 μ K for ⁸⁷Rb. By varying the sensor atom flux into the measurement chamber, controlled by the temperature of the effusive atom source, or the duration of the 3D MOT loading procedure starting from an empty MOT, we can trap anywhere between 10⁶ and 10⁸ lithium or rubidium atoms.

The temperature of the ⁷Li atoms in the 3D MOT is too high for efficient loading into a magnetic trap. To increase efficiency, we decrease the temperature of the gas in the MOT by rapidly changing the detunings of the MOT cooling and repump lasers to $\Delta/\Gamma_{\rm Li} = -1.5$ as well as decreasing MOT cooling laser intensity so that $s_{\rm cool} = 0.1$ and $s_{\rm repump} = 0.05$. This simultaneously increases the atomic density. We operate this "compressed" MOT for 2.5 ms, which reduces the lithium atom temperature to approximately 400 μ K.^{108–110} For rubidium, MOT compression is unnecessary.

D. Optional sub-Doppler cooling stage

If the desired number of atoms in the magnetic trap is $\gtrsim 10^7$, additional cooling is required in order to better match the temperature of the cloud to the maximum trap depths attainable in the magnetic trap. To achieve the requisite temperatures, we use an additional sub-Doppler cooling stage.¹¹¹ For ⁷Li, this stage is Λ -enhanced D_1 grav molasses cooling.^{109,112–118} To begin this stage, the 3D MOT laser beams and the quadrupole magnetic field are rapidly switched off. Simultaneously, laser beams addressing the D_1 transition (${}^2S_{1/2} \rightarrow {}^2P_{1/2}$), generated by a separate amplified external-cavity diode laser, are turned on. Both the cooling and repump light are detuned by $\Delta/\Gamma_{\rm Li} = 3.1$ from the ${}^2S_{1/2}(F = 2) \rightarrow$ ${}^{2}\mathrm{P}_{1/2}(F'=2) \text{ and } {}^{2}\mathrm{S}_{1/2}(F=1) \rightarrow {}^{2}\mathrm{P}_{1/2}(F'=2) \text{ transitional statement of } F'=2)$ sitions, respectively. An EOM generates the repump light to ensure phase coherence with the cooling $light^{109,117}$ and sets the grav molasses cooling-to-repump power ratio equal to 31. The gray molasses beams copropagate with the 3D MOT beams and have the same $1/e^2$ radius, but contain only approximately 12 mW of power, so the gray molasses cooling saturation parameter per beam is $s_{\rm cool} \approx 2.5$. After 2 ms of gray molasses cooling, 25 % of the lithium atoms have been cooled to approximately 20 μ K; the other atoms are lost. The remaining atoms are better temperature matched for efficient transfer into the magnetic trap.

For rubidium, the sub-Doppler cooling stage uses $\sigma^+\sigma^-$ polarization-gradient cooling on the D_2 transition.^{88,119} That is, the 3D MOT quadrupole magnetic field is rapidly turned off, the detuning of the cooling laser is changed to $\Delta/\Gamma_{\rm Rb} = -6.9$, and that of

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Magnetic trap operation E.

We next load the magnetic trap for CAVS operation. We first optically pump all atoms from the ${}^{2}S_{1/2}(F=2)$ hyperfine state into the ${}^{2}S_{1/2}(F = 1)$ state by turning off the repump light and allowing the cooling light to drive the off-resonant $2^{2}S_{1/2}(F=2) \rightarrow 2^{2}P_{3/2}(F'=2)$ transition.^{120–122} This excited F' = 2 state can subsequently decay into the ${}^{2}S_{1/2}(F=1)$ state. This process happens in less than 10 μ s in ⁷Li, as the F' = 2 and F' = 3 states are only partially resolved. For the resolved excited state structure of ⁸⁷Rb, the equivalent process is much slower. We accelerate it by increasing the red detuning of the cooling light from the $2^2 S_{1/2} (F=2) \rightarrow$ $2^{2}P_{3/2}(F'=3)$ transition to $\Delta/\Gamma_{\rm Rb} = -6.9^{123}$ This brings the cooling light slightly closer to the desired $2^2 S_{1/2}(F=2) \rightarrow 2^2 P_{3/2}(F'=2)$ transition, where it is detuned $\Delta/\Gamma_{\rm Rb} \approx +37$. For ⁸⁷Rb, this pumping stage still requires 3 ms, after which most of the atoms are in the F = 1 state. The cooling laser is then tuned to $\Delta/\Gamma_{\rm Rb} = +1$ in order to heat the remaining F = 2 atoms and eject them from the trap within 100 μ s.

We then rapidly change the magnetic field into $\mathbf{B}_{\text{quad}}(\mathbf{x})$ in 2 ms or $\mathbf{B}_{\text{IP}}(\mathbf{x})$ in 3 ms to establish the magnetic trap. Atoms that are locally anti-aligned with the magnetic field (in the projection state M = -1) will be trapped; all others fall out of or are ejected from the trap. The potential energy for these anti-aligned atoms is $V_{\rm trap}(\mathbf{x}) = \mu_{\rm B} |\mathbf{B}(\mathbf{x})|/2 + m_{\rm c} g z$, where the last term represents the non-negligible effect of earth's gravity and q is the earth's local gravitational acceleration. We lose at least 2/3 of the atoms in the transition to the magnetic trap. More atoms are lost due to the lack of spatial mode-matching.³³

We have characterized the transfer of ⁸⁷Rb atoms into the quadrupole and Ioffe-Pritchard magnetic traps: work with ⁷Li is ongoing. For the remainder of this section, we only present results for ⁸⁷Rb. The procedures explained so far lead to at most 5×10^7 , 100 $\mu K^{-87}Rb$ atoms in the magnetic trap. To study collisions among ultra-cold sensor atoms, an important systematic for the CAVS as described in Sec. IIB, we can use this initial condition. For the most accurate pressure measurement, however, we lower the MOT loading time, do not apply sub-Doppler cooling, and reduce the temperature of the atom dispenser to load a much smaller 10^5 to 10^6 atoms into the magnetic trap at 100 μ K.

An important tool both for controlling the effect of sensor atom-atom collisions and for controlling the frac-



FIG. 19. Number of ⁸⁷Rb sensor atoms in a quadrupole trap with $B'_{\text{quad}} = 4.84(2) \text{ mT/cm}$ as a function of time t at our base pressure and vacuum temperature of 295.8(4) K. A fit to our model explained in the text (orange curve) yields loss rates $\beta_2 = 2.7(5) \times 10^{-8} \text{ s}^{-1}$, $\Gamma = 0.0053(1) \text{ s}^{-1}$, and initial atom number $N_0 = 1.16(4) \times 10^5$. All standard uncertainties are statistical. The bottom panel shows the normalized residuals of the fit assuming that the standard uncertainty in the measurement of atom number is $u(N_c) = \sigma_0 N_c$.

tion of glancing collisions during a pressure measurement is the RF knife, which drives transitions between the trapped $|F = 1, M = -1\rangle$ state to the untrapped $|F = 1, M = 0\rangle$ state, to set the depth W of the magnetic trap. Square loop antennas, described towards the end of the introduction of Sec. IV, generate the RF magnetic field at frequency $\omega_{\rm RF}$. For the quadrupole trap, the depth is given by $W = \hbar \omega_{\rm RF}$, neglecting Earth's gravitational pull. For the Ioffe-Pritchard trap, the depth is given by $W = \hbar \omega_{\rm RF} - \mu_{\rm B} B_0/2$, again neglecting gravity. To accurately determine B_0 , given the small day-by-day fluctuating magnetic field in the laboratory, we use the procedure outlined in Ref. 124. Even absent the RF knife, the IP trap has a maximum depth. It is set by the magnitude of the magnetic field at saddle points away from the origin. For our parameters, this maximum depth is about $k \times 400 \ \mu \text{K}$ for ⁸⁷Rb.

As an example of the operation of the ⁸⁷Rb CAVS, we now describe an experiment to measure the base pressure in the first chamber of our dynamic expansion system, estimated to be $\lesssim 10^{-9}$ Pa of pure hydrogen gas. This experiment is done using a weak field gradient of $B'_{\text{quad}} = 4.84 \text{ mT/cm}$, about 60 % larger than the minimum gradient required to support the cloud against gravity. RF radiation is turned on 200 ms after loading the magnetic trap at a frequency of $\omega_{\rm BF}/2\pi = 40$ MHz, corresponding to a trap depth of $W \approx k \times 2$ mK. The frequency is linearly ramped down to $\omega_{\rm RF}/2\pi = 1$ MHz in 1 s, reducing the trap depth to $W \approx k \times 50 \ \mu \text{K}$. The frequency ramp ejects all but the atoms with the low-

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est kinetic energy $E \lesssim k \times 50 \ \mu$ K. After the ramp, the frequency of the RF knife is fixed at $\omega_{\rm RF}/2\pi = 20$ MHz and thus $W \approx k \times 1$ mK. The rate of evaporative atom loss due to elastic collisions between two cold atoms $K_{\rm elas} e^{-W/E}$,⁴³ where $K_{\rm elas}$ is given by Eq. (3). Here, the factor $e^{-W/E} \approx e^{-1/0.05} = 2 \times 10^{-9}$ so that evaporative loss is suppressed.

Figure 19 shows the number of 50 $\mu\mathrm{K}^{125}$ $^{87}\mathrm{Rb}$ atoms N_c in a quadrupole trap as a function of time t under these circumstances. At each t, the atom number is measured by recapturing the remaining atoms into a 3D MOT by turning on the lasers and changing B'_{quad} back to 1.6 mT/cm and counting the atom number through fluorescence photons scattered by the atoms on a camera. This detection is destructive and we must reload the 3D MOT from the atom dispenser and 2D MOT before a new measurement of N_c can be performed.

The data in Fig. 19 are fit to the function

$$N_c(t) = N_0 \frac{\Gamma}{(\Gamma + \beta_2 N_0) e^{\Gamma t} - \beta_2 N_0},$$
 (65)

the solution of Eq. (2) assuming that $\rho_c(\mathbf{x}, t)$ is a product of a function of t and a function of \mathbf{x} , integrating over space \mathbf{x} , and neglecting losses from the Majorana process and three-body recombination, *i.e.* $\gamma = 0$ and $K_3 = 0$. We then find rate $\beta_2 = K_2/\bar{V}$ with initial effective volume for two-body collisions

$$\bar{V} = \frac{\left[\int \rho_c(\mathbf{x}, 0) \mathrm{d}^3 \mathbf{x}\right]^2}{\int \rho_c^2(\mathbf{x}, 0) \mathrm{d}^3 \mathbf{x}} = \frac{N_0^2}{\int \rho_c^2(\mathbf{x}, 0) \mathrm{d}^3 \mathbf{x}}.$$
 (66)

At t = 0, $N_c(0) = N_0$. The fit to Eq. (65) yields lifetime $\tau = 1/\Gamma = 188(3)$ s assuming that the uncertainty in the atom number measurement is $u(N_c) = \sigma_0 N_c$. For $\sigma_0 = 0.058$, we find that the reduced $\chi^2_{\nu} = 1$ and the normalized residuals $|N_c(t) - N_{\rm fit}(t)| / \sigma_0 N_c$ are random, and thus independent of N_c , with unity standard deviation, as shown in the bottom panel of Fig. 19. This linear dependence of $u(N_c)$ on N_c is due to technical fluctuations in the experiment, which cause the initial atom number to fluctuate by 5 %.

The fitted value for β_2 is surprisingly large and can not be explained with the ⁸⁷Rb two-body inelastic rate coefficient of $K_2 = 1.6 \times 10^{-14} \text{ cm}^3/\text{s}$ given in Sec. II. For our atom number and temperature $V \approx 2.3 \times 10^{-2}$ cm³. Thus, our fitted K_2 from $\beta_2 = 2.7(4) \times 10^{-8} \text{ s}^{-1}$ is on the order of $10^{-10} \text{ cm}^3/\text{s}$, four orders of magnitude larger that the expected two-body loss rate due to inelastic collisions. An investigation of this anomalously large value of β_2 is in progress.

The pressure, as determined by the ⁸⁷Rb CAVS, can be calculated with the Eq. 1, where T = 295.8(4) K is the temperature of the background gas, $\Gamma = 0.0053(1) \text{ s}^{-1}$ is the measured loss rate, and $L_{\rm H_2} = 4.9(1.2) \times 10^{-9} \text{ cm}^3/\text{s}$ is the ⁸⁷Rb+H₂ semi-classical rate coefficient given by Eq. (11). We estimate a pressure of 4.3(1.1) nPa, where

MOT **Diffraction Grating** Differential Pumping Tube Dispenser Magnet Holder NEG FIG. 20. A computer-assisted-design rendering of one of

Magnets

our portable cold-atom vacuum standards (pCAVS). The red and blue coloring of the 3.81 cm long magnets indicates the relative orientation of their poles. The source chamber is pumped by a non-evaporable getter (NEG). Reproduced from L. H. Ehinger, B. P. Acharya, D. S. Barker, J. A. Fedchak, J. Scherschligt, E. Tiesinga, and S. Eckel, AVS Quantum Science 4, 034403 (2022), public domain.

the dominant uncertainty is an assumed 25 % uncertainty in the semiclassical estimate of $L_{\rm H_2}$. The fraction of glancing collisions $P_{\rm gc}$, given by Eq. (29), is about 0.06 and small compared our final uncertainty.

V. PORTABLE PRESSURE STANDARD (PCAVS)

NIST has also developed a portable pressure sensor based on the same operating principles as the laboratory CAVS described in Section IV. Using ⁷Li sensor atoms, this portable CAVS (pCAVS) is significantly smaller, less complex, and less costly than the laboratory CAVS. Figure 20 shows a computer-assisted-design rendering of our prototype pCAVS. Built around a 7 cm stainless steel cube and requiring only a single input laser beam, the pCAVS is designed to replace an ionization gauge. Recently, we demonstrated the simultaneous operation of two pCAVSs measuring the pressure in a chamber evacuated to a UHV pressure.¹²⁶ Their pressure readings at 41.8 nPa agree to 1.6 %.

The pCAVS has a source chamber where a dispenser effuses lithium atoms into the vacuum and a measurement chamber where those atoms are laser cooled and trapped, loaded into a magnetic trap, and probe the vacuum pressure. The two chambers are separated by a differential

Magnets

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pumping tube of length 26.7 mm and radius 1.5 mm. This tube has a computed conductance of 0.014 L/s for N_2 at 300 K based on Eqs. (33) and (34).

Our current commercial alkali-metal dispenser (AMD) effuses lithium atoms into the source chamber when heated. A current between 5 A to 7 A runs through the AMD, resistively heating it to temperatures between $350 \,^{\circ}$ C and $450 \,^{\circ}$ C. The opening of the AMD is pointed such that the direction of maximum lithium atom flux is aligned with the long axis of the differential pumping tube. The AMD, however, outgasses species other than lithium, including molecular hydrogen and nitrogen. Such gases are pumped away using a non-evaporable getter pump (NEG), rated at 100 L/s for H₂. In Sec. V D, we describe alternative lithium source technologies that suffer less from unwanted outgassing and might be used in next generation pCAVSs.

In the measurement chamber, a specially designed nanofabricated diffraction grating chip is used to slow, cool, and trap the hot ⁷Li atoms passing through the differential pumping tube with a single laser beam.³⁶ This chip shrinks 2 m^3 of optics down to a single fiber launch, and also allows us to shrink the vacuum enclosure to about twice the volume of a standard ionization gauge. The pCAVS typically traps 10^5 ⁷Li atoms in the grating MOT (gMOT) that forms above the grating chip. This is about a factor of 100 less than in the 3D MOT of the laboratory CAVS, but more than adequate to obtain single-shot counting statistics below our 2 % systematic uncertainty of the pCAVS, as will be described below. Section VA briefly describes the challenges of miniaturizing a Li laser-cooling system and a test apparatus used to verify slowing and trapping into the 3D grating MOT. Sections VB and VC describe the optical properties of and manufacturing process for the grating MOT chip, respectively.

The quadrupole magnetic field for the 3D grating MOT and subsequent quadrupole magnetic trap is generated using type-N52 NdFeB permanent magnets. The axial magnetic field gradient is $B'_{\text{quad}} = 7.53(28) \text{ mT/cm}$ and the trap depth of the magnetic trap is W/k = 1.5(3) mK for ⁷Li. The facts that the axial field gradient is the same for the 3D MOT and magnetic trap and that there is no need for RF loop antennas to create the RF knife simplify the design when compared to that of the laboratory CAVS described in Sec. IV. Laser light is generated by a single amplified external-cavity diode laser, detuned by $\Delta_{\rm Li}/\Gamma_{\rm Li} = -2$ from the ${}^{2}{\rm S}_{1/2} (F = 2) \rightarrow {}^{2}{\rm P}_{3/2} (F' = 3)$ transition. As with the laboratory CAVS, an EOM tuned to 813 MHz generates two sidebands with approximately 50 % of the power of the carrier, the blue sideband being detuned by $\Delta_{\rm Li}/\Gamma_{\rm Li} = -2$ from the ${}^2S_{1/2}(F=1) \rightarrow$ ${}^{2}\mathrm{P}_{3/2}(F'=2)$ transition.

The procedure for loading the magnetic trap is similar to that for the laboratory CAVS. The gMOT is loaded for approximately 3 s, after which it contains about 10^5 ⁷Li atoms cooled to about 750 μ K. The EOM is subsequently turned off and the ⁷Li atoms are optically pumped into



FIG. 21. Recaptured ⁷Li atom number N/N_0 as functions of time t in the magnetic quadrupole trap. The example decays were recorded before (a) and after (b) a leak in pCAVS #1 was fixed; note the difference in time scales. Blue circles and red squares are for pCAVS #1 and pCAVS #2, respectively. Solid lines show fits assuming exponential decay. The error bars on the markers correspond to the standard error in the mean. Reproduced from L. H. Ehinger, B. P. Acharya, D. S. Barker, J. A. Fedchak, J. Scherschligt, E. Tiesinga, and S. Eckel, AVS Quantum Science 4, 034403 (2022), public domain.

the F = 1 hyperfine ground state. To maintain design simplicity, we do not use the gray molasses cooling step for the pCAVS, which would require an additional laser.¹²⁷ Hence, only one-tenth of the atoms are both cold enough and in the trappable $|F = 1, M = -1\rangle$ hyperfine state to be captured by the magnetic trap. The magnetic trap initially has about 10^4 atoms.

The ⁷Li atoms are held in the quadrupole magnetic trap for a variable amount of time and then recaptured into the gMOT to count the remaining number of atoms. Figure 21 shows the time-evolution of the ⁷Li atom number for two pCAVSs, pCAVS #1 and pCAVS #2, that are connected to the same independent vacuum chamber, and therefore should measure the same pressure. We show the number of atoms recaptured in the gMOT Ndivided by the number of atoms captured in the initial gMOT N_0 as functions of time in the magnetic trap t. This ratio is less sensitive to the effects of fluctuations in the atom number. In Fig. 21(a), the measured decay rates of the two pCAVS differ significantly, because of a small leak in a viewport attached to pCAVS #1. The leak's throughput was of the order of 10^{-6} Pa L/s. small enough to evade detection with a residual gas analyzer using a Faraday cup detector. After the leak was repaired, the two pCAVS do indeed measure essentially the same decay rates, as shown in Fig. 21(b). In fact, the
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corresponding and consistent pressures, assuming a background gas of H₂, are 41.5(1.2) nPa for pCAVS #1 and 42.2(1.0) nPa for pCAVS #2. The quoted uncertainties are dominated by the 2% uncertainty in the theoretical value for $L_{\rm H_2}$ found in Eq. (30). The next largest contributors to the uncertainties, in order of importance, are the statistical noise in N/N_0 , possible Majorana losses at the center of the quadrupole trap, and the uncertainty in the fraction of glancing collisions $P_{\rm gc}$. The semiclassical expression for $P_{\rm gc}$ is given in Eq. (29). Further details about the uncertainty budget can be found in Ref. 126.

A. Test apparatus for miniaturized cooling and trapping of ⁷Li atoms

Miniaturizing the ⁷Li cooling apparatus poses different challenges compared to those for other commonly laser cooled atoms, such as ⁸⁷Rb. The loading rate $R_{\rm MOT}$ of a MOT scales as $(v_c/v_p)^4$, where v_c is the MOT capture velocity defined in Eq. (62) and $v_p = \sqrt{2kT_{\rm S}/m}$ is the most probable thermal velocity for atoms of mass m effusing out of the AMD at temperature $T_{\rm S}$. The ratio v_c/v_p is independent of mass. Then inspection shows that the primary difference in v_c/v_p for ⁷Li and ⁸⁷Rb is $T_{\rm S}$, which are 700 K and 300 K, respectively. Thus, lithium should have five times lower loading rates than rubidium.

Rubidium has a further advantage over Li. Lithium atoms effusing out of the AMD that are not captured by the MOT stick to the walls of the room temperature vacuum chamber with near 100 % probability, a direct consequence of its low saturated vapor pressure of 10^{-17} Pa at room temperature. On the other hand, rubidium atoms that are not immediately captured by the MOT can bounce of the chamber walls, given its much larger saturated vapor pressure of 2×10^{-5} Pa. Thus, most rubidium atoms get multiple chances to be captured by the MOT. These geometry considerations further limit the achievable ⁷Li loading rate into a MOT.

We overcome these difficulties by designing a short ⁷Li Zeeman slower to be operated in conjunction with our custom grating MOT chip that optimizes the capture velocity of the combined gMOT/Zeeman slower system. Zeeman slowers use a single laser beam that opposes the momentum of the atoms as they are emitted from the source, and a spatially dependent magnetic field along this direction. The magnetic field profile is designed such that the atomic transition frequency including Zeeman shifts stays close to resonance with the laser frequency in the gMOT/Zeeman slower system. For example, assuming the constant acceleration at every point in space, the most efficient field profile is $B(z) \propto \sqrt{z}$, where the atoms will come to a standstill at $z = 0.^{88}$ Many B(z) profiles will work, however, provided that the change in the Zeeman shift does not exceed the change in the Doppler shift of the decelerating atom at any point along the atomic trajectory.³⁶ In our combined gMOT and slower, the magnetic field along the axial z direction goes through

zero at the center of the gMOT, and has a maximum $B_{\rm max}$ between the gMOT and the effusive source. The resulting capture velocity of the gMOT/Zeeman slower system is given by $v_{\rm S} = \mu_{\rm B} B_{\rm max}/\hbar k_{\rm L}$, which is the maximum velocity that can be shifted into resonance for cooling by the Zeeman slower.

We tested our combined gMOT and slower in a standalone apparatus, described in Ref. 36. In fact, the experiments with this test apparatus were conducted before we designed our first-generation pCAVS. In the test apparatus, shown in Fig. 22(a), the gMOT chip is centered between several electromagnets. The design of the chip will be described in detail in Sec. VC. An input laser beam strikes the grating MOT chip, creating three reflected beams that intersect with the input beam, making the minimum four intersecting beams that are required for stable MOT operation just above the chip. A portion of the input beam proceeds through the triangular hole in the center of the chip and strikes the output of the effusive source, placed 49 mm beyond the chip with its preferred emission direction pointed toward the triangular hole in the chip. This light acts as the laser beam for the Zeeman slower.

In-vacuum electromagnets in the test apparatus tailor the spatial profile of the magnetic field for for the combined gMOT and Zeeman slower. In the pCAVS, permanent magnets located outside the vacuum system create these fields. The test apparatus has two anti-Helmholtz coils, called the "MOT coil pair", of mean diameter 3.89 cm and separated by 3.15 cm, which generate the $B'_{\text{quad}}(-x/2,-y/2,z)^T$ quadruple field for the MOT. Here, the axial direction of the coil assembly is our z axis. This expression for the magnetic field is only valid within a radius of 1 cm from the center of the MOT at (x, y, z) = (0, 0, 0). Of most concern for us is that along the axial direction with (x, y) = (0, 0)the z-component of the magnetic field reaches a maximum $B_{\text{max}} \approx 7 \text{ mT}$ near either one of the MOT coils. A "Zeeman slower coil" and a "slower compensation coil", positioned around the MOT coils, extend the z range over which $B_z = B'_{quad} z$ is valid and increase to at most $B_{\rm max} \approx 13 \text{ mT}$, now located near the Zeeman slower coil. The larger $B_{\rm max}$ should increase the capture velocity $v_{\rm S}$ of the combined gMOT and Zeeman slower by almost a factor of two. Moreover, naively the gMOT loading rate $R_{\rm MOT} \propto (v_c/v_p)^4 \propto B_{\rm max}^4$ and is independent of $B'_{\rm guad}$ based on integrating the velocity probability distribution from the effusive source in Eq. (61) from v = 0 to $v_{\rm S}$ with $v_{\rm S} \ll v_p$. We thus naively expect the Zeeman slower coil to increase the gMOT loading rate by about a factor of 16. "Blossoming" of the slowed atomic beam, a divergence of the atomic beam due to the unslowed transverse velocity, however, limits $R_{\rm MOT} \propto B_{\rm max}^3$.³⁶

Figure 23 shows the efficacy of our mini-gMOT/slower as measured in the test apparatus. Here, loading rates $R_{\rm MOT}$ are shown as a function $B_{\rm max}$ for four axial quadrupole field gradients $B'_{\rm quad}$. The data suggests a scaling of $R_{\rm MOT} \propto B^2_{\rm max}$, slower than the expectation of This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset

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Apparatus for testing the grating chip for ⁷Li FIG. 22. atoms. (a) Photograph of the test apparatus before insertion into its vacuum chamber. It has three individual electromagnets: A "slower compensation coil", a "MOT coil pair", and a "Zeeman slower coil", labeled by (1), (2), and (3), respectively. The chip is rigidly mounted between the coils of the MOT coil pair, oriented in the same plane as these coils, and with the grating pointing towards the slower compensation coil (1). In this picture, the input laser beam comes from the top of the image traveling downward. The MOT for the Li atoms forms above the chip. The Li dispenser, not visible in this view, is mounted below the Zeeman slower coil (3). (b) Photograph of the triangular grating chip with a 24 mm diameter US quarter dollar for scale. (c) Scanning electron micrograph of the chip near one of the vertices of the triangles and the central triangular hole. (d) Side image of the grating showing the aluminum layer (white area) deposited on a silicon surface (gray area). Trench depth, period, and aluminum layer thicknesses of the grating are indicated. Reproduced from D. Barker, E. Norrgard, N. Klimov, J. Fedchak, J. Scherschligt, and S. Eckel, Phys. Rev. Applied 11, 064023 (2019), public domain.

 B_{\max}^3 due to blossoming, and a smaller dependence on B'_{quad} that decreases with B'_{quad} . A numerical model of the slowing process for a $F = 0 \rightarrow F = 1$ atom is presented in Ref. 36 and is shown as the curves in Fig. 23. The model includes a small, fitted 2.5 mm transverse lateral displacement of the source that further reduces the scaling power. The misalignment is also responsible for the dependence on B'_{quad} . Despite the imperfections, we nevertheless conclude that use of our Zeeman slower outperforms other potential gMOT and source configurations, including placing the effusive source anywhere above the plane of the gMOT chip.

B. Optical properties of the grating MOT chip

In this section, we describe the optical properties of the gMOT chip. The grating consists of concentric equi-



FIG. 23. Loading rates $R_{\rm MOT}$ of the ⁷Li gMOT (markers with standard uncertainties) as functions of maximum magnetic field $B_{\rm max}$ encountered by the atoms in the test apparatus of Fig. 22 for four axial quadrupole field gradients: 4 mT/cm (blue), 4.5 mT/cm (orange), 5 mT/cm (green), and 5.5 mT/cm (red). Solid curves are fits to the data with a numerical model of the laser cooling process described in Ref. 36. Adapted from D. Barker, E. Norrgard, N. Klimov, J. Fedchak, J. Scherschligt, and S. Eckel, Phys. Rev. Applied **11**, 064023 (2019), public domain.

lateral triangles, cropped to a circle of 22 mm diameter, etched into silicon with a convenient spatial period of 1.00(1) μ m. The first-order diffraction angle is then $\approx 42^{\circ}$ for laser light at the D_1 and D_2 ⁷Li transition wavelengths of $\lambda_{\rm Li} \approx 671$ nm. An aluminum layer with a thickness of 100(5) nm on top of the etched silicon leads to a measured 37(1)% first-order diffraction efficiency, close to the optimal 33 % efficiency for balanced intensities of light going toward and diffracted away from the $chip.^{128}$ Figure 22(c) shows a scanning electron micrograph (SEM) image of the triangular grating near a vertex of the central triangular hole that is etched through the chip. The light from the input beam that passes through the hole forms the Zeeman slower beam, described in Section VA. Figure 22(d) shows a cross section of just over a period of the grating obtained by cleaving a chip orthogonally to the lines of the grating and imaging the side with SEM. The length and depth of the trenches are indicated in the figure and the aluminum top layer is clearly visible. The 168(2) nm trench depth is designed to be close to $\lambda_{\rm Li}/4$ in order to minimize reflection back into the input beam direction.

The Q, U, and V Stokes parameters¹²⁹ for the polarization of the reflected light from grating, assuming a left-circularly polarized input beam with wavevector $k_{\rm L}$ normal to the plane of the grating chip, are Q = 0.16(1), U = -0.37(1), V = 0.92(1). Here, we use the coordinate system where Q = 1 corresponds to linear polarization in the plane spanned by the incident and reflected wavevectors and Q = -1 corresponds to linear polarization perpendicular to the same plane.

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C. Fabrication of the grating MOT chip

In this section, we describe the fabrication of the gMOT chip, which was performed at the Center for Nanoscale Science and Technology clean room facility of the National Institute of Standards and Technology. Fabrication of the gMOT chip starts with a commercially-available, single-side polished 525 μ m-thick prime Si (100) wafer of diameter 100 mm. It ends with a wafer containing four gMOT chips, each of size $27.0 \text{ mm} \times 39.0 \text{ mm}$, as shown in Fig. 24. The fabrication process has three main steps: (1) the fabrication of a shallow nanoscale grating on the polished side of the wafer, (2) the fabrication of the etch-through central triangular aperture, and (3) an aluminum thin film deposition on top of the Si grating. We use aluminum, but the process can be adapted to other highly reflective metals, e.g. silver or gold. Notation, e.g. the chip's reference name and/or logo, can be imprinted on the chip's surface via an additional lithography step and a shallow Si etch between steps (1) and (2). All lithography and etch steps are performed on the polished side of the wafer. Before the start of each nanofabrication step, we clean each wafer with a Standard Clean 1 $(SC-1)^{130}$ process to remove organic contaminants from wafer surface. In our fabrication procedure, we process a batch of 25 wafers at the same time with a near 100% fabrication yield.

The first nanofabrication step defines a set of four concentric triangular gratings each trimmed to a circle with a diameter of 22.0 mm on the Si wafer. The grating pattern is lithographically defined in photoresist and transferred into Si with a dry plasma etch. To control this first highresolution photolithographic step and to avoid standing wave interference within the photoresist to be used in the direction orthogonal to wafer surface, we begin by spincoating a bottom anti-reflective coating (BARC), WiDE-8C from Brewer Science, on the polished and cleaned Si wafer surface. The BARC layer minimizes backreflection of the i-line ultraviolet (UV) light (corresponding to a wavelength of about 365 nm) used during lithographic exposures. Furthermore, WiDE-8C and photoresist are simultaneously wet-developed in a tetramethylammonium hydroxide (TMAH) solution, which is possible given the bake conditions described below. WiDE-8C eliminates the need for additional dry etching after photoresist development to fully define a soft etch mask.

In order to improve the wettability of the silicon surface and promote the uniform adhesion of WiDE-8C to silicon, prior to BARC spin-coating, the polished silicon surface is functionalized from hydrophobic to hydrophilic by an oxygen plasma exposure for 2 minutes operating at 700 W RF power with O_2 flow rate and pressure of 600 standard cubic centimeter per minute (sccm) and 1.3 Pa, respectively. After the plasma treatment, we spin-coat the BARC layer at 2750 rpm for 60 s, leading to a 75(3) nm thick BARC film, as measured by ellipsometry. At this thickness, the backreflectance of the i-line UV is less than 2%. Subsequently, we bake



FIG. 24. Wafer layout for grating magneto-optical traps. The black mostly circular curve shows the edge of the 100 mm diameter Si wafer with four grating chips in its center. Green and blue features are defined in lithographic steps (1) and (2), respectively. The green regions are the diffraction gratings. The green squares and plus symbols surrounding each of the green areas are alignment marks. The blue triangles are the central apertures. The thin blue lines ending in blue circles are 50 μ m wide chip separation lines. These circular end points do not touch, leaving 70 μ m anchor points between them (not resolved). The red identifying notation can be added to the wafer in an optional lithographic step between steps (1) and (2).

on two hotplates: first, at 100 °C for 30 s, and then at 167 °C for 60 s. Next, we spin-coat MEGAPOSIT SPR 220-1.2 i-line photoresist over the baked BARC layer at 2000 rpm for 60 s and baked on a hotplate at 115 °C for 90 s. The resist thickness of 1220(20) nm, as measured by ellipsometry, is sufficient for transferring the developed photoresist pattern into Si during the dry plasma etch process.

The lithographic exposure is performed on an ASML PAS 5500/275D i-line stepper using 365 nm ultraviolet light and a reticle containing the concentric triangular grating. We use the stepper's $5 \times$ reduction and projection capabilities with step and repeat to transfer the reticle pattern to four locations on the wafer. The diffraction grating design, overlaid on a wafer outline, is shown in green in Fig. 24. In addition to the triangular grating, this first step of lithography also contains 22.0 mm by 22.0 mm squares that enclose the grating patterns, close to the edge of the single write-field size of the stepper. By confining the triangular grating to a single write-field, we avoid stitching errors. Finally, this first step of lithography also defines five crosses: four in the corners of the write field boundary and one in the center of the triangular pattern (not shown on the image). These crosses

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are later used as fiducial marks to align subsequent lithographic exposures relative to the first pattern.

The grating period on the reticle is $5.00(1) \ \mu$ m, which, given the 5× stepper reduction, leads to the desired $1.00(1) \ \mu$ m period on the wafer. The spatial duty cycle of the grating on the reticle is 0.50 % less than the desired duty cycle of the grating on the chip, to account for the widening of clear openings of a positive photoresist mask during pattern exposure and further development of the wafer. The pattern exposure dose is $110 \ \text{mJ/cm}^2$ with no focus offset relative to the resist surface. This exposure dose will lead to a 60 % spatial duty cycle of the grating in the silicon after etching, corresponding to a 600(5) nm trench width. By varying the exposure dose from this nominal value, we can achieve spatial duty cycles ranging from 50 % to 70 %.

Following the pattern exposure, a bake is performed on a hotplate at 110 °C for 90 s. Afterwards, both BARC and photoresist layers are developed in AZ 300 MIF, containing less than 3 % TMAH by weight, at room temperature for 60 s with gentle manual agitation of the wafers. Subsequently, the wafers are rinsed, first in this developer diluted with deionized water (DIW) at a ratio of 1 to 10 by volume for 60 s, and then a rinse in only DIW for 60 s. The rinsed wafers are dried under N₂ gas.

The triangular grating formed in photoresist is transferred into silicon via inductively coupled reactive ion plasma dry etching (ICP RIE) using an Oxford Plasmalab 100 etcher. The first step of this process is to remove any undeveloped resist using an O_2 plasma for 30 s with the following parameters: O_2 flow rate of 100 sccm at 2 Pa pressure, DC power of 25 W, RF power of 500 W, and etch chamber temperature of 30 °C. Following this "descum", we etch silicon in a pseudo-Bosch process in a gas mixture of SF_6 and C_4F_8 . The flow rates for SF_6 and C_4F_8 are 33 sccm and 57 sccm, respectively. Gas pressure is maintained at 2 Pa, temperature at 15 °C, DC power at 15 W, and RF power at 3000 W. Under these plasma conditions the silicon etch rate is approximately 6.5 nm/s. Depending on the desired final trench depth of the grating, the etch depth of Si grating is chosen to be anywhere from 163 nm to 190 nm. This range spans the optimal trench depth for both ⁷Li, shown in Figure 22(d), and ⁸⁷Rb. After the etch, the remaining photoresist mask is removed in an O_2 plasma using the same parameters as before. This completes the first step of lithography. To imprint notation on the wafer, such as the chip's name, index, and logo, the fabrication step (1) can be repeated with the appropriate reticle.

The second lithographic step creates the central equilateral triangular apertures with a smallest enclosing circle of 3 mm radius, the 50 μ m wide separation lines with circular endpoints shown in blue in Fig. 24. The circular endpoints do not touch each other, leaving 70 μ m anchor points points between them, which allow for easy cleaving of the four gMOT chips out of the wafer. For this second photolithography step, after the obligatory SC-1 cleaning, we prime the wafers with hexamethyldisilazane vapor to improve the adhesion of photoresist for the next lithographic step.

We then spin coat 10XT-520cP photoresist at 4000 rpm for 60 s, followed by a hotplate bake at $110 \,^{\circ}\text{C}$ for 180 s. The resulting 7.3 μ m thickness of the photoresist meets the manufacturer's specification, confirmed by ellipsometry measurement. The design pattern for this lithographic step is transferred into the photoresist on a Heidelberg MLA-150 direct laser writer. We expose the pattern with a 1000 mJ/cm^2 dose of g-line light, corresponding to a wavelength of 436 nm, with no focus offset relative to the resist surface. This is followed by, first, a delay of 2.5 h to stabilize the resist, and then a bake performed on a hotplate at 110 °C for 90 s. We develop the pattern in AZ 300 MIF developer for 8 minutes, rise in DIW for 60 s, and dry with N_2 gas. To harden the resist mask, we bake the developed wafers in a vacuum oven at 95 °C for 3 h and then expose to broadband UV light for 15 min at 90 °C.

The through-wafer etch is performed in a deep Si ICP RIE etcher made by Unaxis Shuttleline DSEII using the Bosch process.¹³¹ After etching $\approx 120 \ \mu m$ of Si, the process is interrupted for 10 min to cool the substrate. For the last 100 μm of the etch, the wafer is placed on top of a 100 mm diameter Si carrier wafer to prevent damage of the tool once the pattern has fully etched through. After the completion of the etch, the four chips are snapped from the wafer by breaking the four anchor points on each chip. This avoids wafer dicing. The remaining photoresist mask on each cleaved chip is removed in an O₂ plasma with parameters as used in the first fabrication step.

The third and final fabrication step is metal deposition. A 4Wave IBD/BTD Cluster Sputter system deposits a 5.0 nm layer of titanium followed by a 100(5) nm layer of aluminum. During the metal deposition, the deposition rate on the vertical sidewalls of the trenches is two times slower than the deposition rate on the horizontal surfaces as shown in Fig. 22(d). To achieve a 50 % spatial duty cycle for the metallized grating, therefore, the exposure dose during the first photolithography step was chosen to achieve a Si grating with a 60 % spatial duty cycle, corresponding to a 600 nm trench width. After sputtering Ti and Al, the width of the trenches narrows by 100(5) nm and the spatial duty cycle is reduced to 50 %.

D. Alternative lithium sources

Operation of the pCAVS perturbs the vacuum slightly. The pCAVS experiments described in Ref. 126 observed a pressure rise of about 1.0 nPa under typical conditions. The ≈ 300 °C stainless-steel walls of the commercial AMD used in those experiments lead to non-negligible outgassing of H₂ into the pCAVS and is a possible cause of the pressure rise. In order to extend the operation of the pCAVS into the XHV regime, lower-outgassing alkali metal sources may be required. (In our laboratory-based

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FIG. 25. A picture of the 3D-printed titanium alkali metal dispenser. Its "plug", shown on the left, fits snuggly into the open end of its "tube", shown on the right. Tabs with clearance holes on both parts are used for mounting and electrical connections. A ruler is included for scale. Figure reproduced from E. B. Norrgard, D. S. Barker, J. A. Fedchak, N. Klimov, J. Scherschligt, and S. Eckel, Rev. Sci. Instrum. **89**, 056101 (2018), public domain.

CAVS with its separate source and vacuum measurement chambers, each with large pumping speed, connected by a narrow differential pumping tube, this outgassing by the dispenser is much less relevant.)

We have tested two new sources for lithium atoms to replace the commercial dispenser in our current lithiumbased pCAVSs. The dispensers are designed to have significantly smaller outgassing rates. They are a 3Dprinted titanium dispenser and a source based on laserinduced desorption of lithium from a surface near the magneto-optical trap of the pCAVS. In this subsection, we describe these devices in more detail.

1. 3D-printed Ti source

The commercial atom source may be replaced by a direct-metal-laser-sintered (DMLS) titanium dispenser.¹³² This source is resistively heated in the same manner as our commercial dispenser to form an effusive beam of Li atoms. Titanium, however, is a low-outgassing, XHV-compatible material.

Our DLMS titanium dispenser is shown in Fig. 25 and has two parts: a tube with a 5.1 mm diameter, a 13.8 mm length, and a 0.13 mm wall thickness and a plug with a 1.2 mm thickness that snugly fits into the open end of the tube. Both the tube and plug have 0.25 mm thick, 5.1 mm wide tabs with a 2.4 mm diameter clearance hole for mounting and electrical connections. In addition, a 5.1 mm long, 0.25 mm wide slit in the tube allows the lithium atoms to effuse from the AMD. The tube and plug have a measured combined mass of 584(2) mg and a designed total surface area of 6.8 cm². This AMD holds roughly 100 mg of solid Li with natural abundances of its two stable isotopes.

In tests of the titanium dispenser operating at a temperature of ≈ 330 °C, outgassing throughputs of $q \lesssim$

 5×10^{-7} Pa L s⁻¹ are observed. These throughputs are about a factor of 20 times lower than those from the commercial AMD at the same operating temperature. The primary contaminant from operating the titanium source is now N₂ rather than H₂. This is attributed to the formation of a nitride layer on the lithium pellets when interacting with air during source loading. By loading the source in an inert gas or vacuum environment, the N₂ contaminant could likely be reduced.

2. Light-induced atomic desorption of lithium

The second low-outgassing dispenser is based on lightinduced atomic desorption (LIAD), and is described in detail in Ref. 133. Here, a coating of alkali-metal atoms is prepared on a vacuum surface, typically a nearby vacuum viewport. Such coatings often occur when operating an AMD for long periods of time, but can also be intentionally prepared by directing the effusive alkali-metal beam from a commercial AMD at a vacuum surface. The AMD is then turned off and cooled down, minimizing outgassing of H₂. The alkali-metal atoms can then be desorbed from the vacuum surface by incident light from light-emitting diodes (LEDs) with blue or ultraviolet (UV) wavelengths.¹³³

We have tested the LIAD-based dispenser of ⁷Li by characterizing the loading of a standard six-beam MOT in an auxiliary vacuum chamber when an LED is turned on. We load the 3D MOT for 40 s and the atom number is seen to saturate. The loading curve is nontrivial as we observe that the pressure p in the chamber rises above the baseline vacuum level by as much as 50% in about 30 s. We fit the loading curve to a function that, among others, has a UV-wavelength and power dependent loading rate R_{MOT} and a pressure-dependent atom loss rate $\Gamma = Lp/kT_{\text{chamber}}$.¹³³ Figures 26(a) and (b) show the measured atom number $N_{\rm e}$ at t = 40 s and fitted $R_{\rm MOT}$ as functions of LED power and their "peak" wavelength, respectively. Here, we have used LEDs with a light spectrum that peak at wavelengths of 445 nm, 405 nm, and 385 nm.

For all three LEDs, $N_{\rm e}$ and $R_{\rm MOT}$ increase linearly with LIAD power, although saturation of the equilibrium number of atoms with LIAD power might have been reached for the LEDs with a peak wavelength of 405 nm and 445 nm. In addition, we observe that both $N_{\rm e}$ and $R_{\rm MOT}$ are larger for smaller peak LED wavelengths, suggesting that faster loading rates could be achieved with a deeper-UV LED. LIAD-loaded MOTs of other alkali-metal species exhibit consistent behavior,¹³⁴ but unlike for other alkali-metal species, ⁷Li LIAD-based MOT loading is inferior to that of loading with an AMD. LIAD-loaded ⁷Li MOTs with up to 4×10^4 atoms were observed. Additionally, for the fastest loading rate of $R_{\rm MOT} = 4 \times 10^3 \, {\rm s}^{-1}$ MOT loading times are long at 10's of seconds.

The primary advantages of operating a pCAVS with

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LIAD loading are source longevity and reduced power requirements. An alkali-metal atom dispenser takes a few minutes to resistively heat from ambient to operating temperatures, while continually dissipating 3W of power. This minutes delay means that the dispenser is typically maintained at operating temperature between CAVS pressure measurements. In addition, this implies that Li atoms are always effusing from the AMD, and those not trapped by the MOT are effectively lost. For LIAD loading, atoms need only be desorbed from the vacuum surface when required by applying an optical power of 1 W for at most tens of seconds. Lithium atoms liberated by LIAD, but not trapped by the MOT will stick to another surface, allowing for the potential for LIAD to liberate them again. Moreover, the AMD only needs to be heated up when all atoms have been desorbed from the surfaces. For measurement of vacuum pressures $< 10^{-8}$ Pa, where the corresponding vacuum lifetimes are > 100 s, it is clear that LIAD presents an energy efficiency advantage.

VI. CONCLUSION

We have given an overview of the technical aspects - the design, construction, and modelling - of the coldatom vacuum standard (CAVS) for measuring pressure in the ultra-high (UHV) and extreme-high vacuum (XHV) domain. Developed at the National Institute of Standards and Technology, this effort is a mix of vacuum metrology and atomic and molecular physics. Its operating principle, measuring the loss rate of ultra-cold. sub-millikelvin sensor atoms from a shallow magnetic trap due to collisions with room-temperature background atoms and molecules, is deceptively simple. Sensor atoms are typically alkali-metal atoms as they can be routinely cooled to the required temperatures. Translating the loss rate into a better than a few percent vacuum pressure measurement requires quantum scattering calculations of fundamental loss rate coefficients, eventually confirmed by experimental data. These loss rate coefficients are immutable, the same in everywhere in the world, and thus the CAVS represents a *primary* standard of vacuum. It is a calibration-free standard of pressure.

We began the review by explaining the theoretical underpinnings of the collisional processes relevant for the CAVS. A collision that imparts only a little momentum or kinetic energy to a sensor atom is already sufficient to remove this atom from its magnetic trap. The likelihood of sufficient momentum transfer is largest for the lightest sensor atoms and can be described in terms of small-angle scattering. In fact, a semi-classical model that only requires knowledge of the van-der-Waals interaction between the colliding partners is sufficient to predict rate coefficients to $\sim 10\%$. For better than a few percent accuracy quantum mechanical calculations are required. We review our quantum simulations for $^{7}Li+H_{2}$ collisions, as molecular H₂, desorbing from the vacuum





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(a)

FIG. 26. Loading characteristic of a ⁷Li magneto-optical trap using lithium that has been desorbed from the walls of the vacuum chamber by light-induced atomic desorption (LIAD). (a) Measured equilibrium number of atoms $N_{\rm e}$ loaded into the MOT as functions of LIAD optical power emitted by LEDs operating at one of three peak wavelengths. Blue squares, magenta triangles, and pink circles are data for LEDs with peak wavelengths of 445 nm, 405 nm, and 385 nm, respectively. (b) Fitted loading rates R_{MOT} of atoms into the magneto-optical trap as functions of LIAD optical power for the same three LEDs as in panel (a). The black lines are linear fits to the fitted R_{MOT} . In both panels error bars represent standard statistical uncertainties. Figure adapted from D. S. Barker, E. B. Norrgard, J. Scherschligt, J. A. Fedchak, and S. Eckel, Phys. Rev. A 98 043412 (2018), public domain.

chamber walls, is the dominant gas species present at UHV pressures and below.

We then discussed the challenges of vacuum metrology in the UHV regime. Vacuum metrology in this regime requires chamber walls made of low-outgassing materials. We discussed material choices as well as heat treatments that eliminate contaminants adhering to chamber walls or absorded in the walls. For the CAVS, we chose titanium and 400 °C-baked stainless steel. We also described the construction of a novel dynamic expansion and flowmeter system. It allows for the generation of partial pressures from 10^{-8} Pa to 10^{-6} Pa, with better than 1 % uncertainty and will, in the future, be used validate the theoretical underpinnings of the CAVS. Partial pressures as low as 10^{-10} Pa, extending into the XHV regime, can be achieved with an optional flow splitter,

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is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0120500 albeit with anticipated uncertainties of a few percent. These advances rely on a flowmeter that is capable of generating and measuring flows as small as 10^{-13} mol/s.

Next, we described our laboratory-based CAVS and showed that we can measure an ultra-high vacuum of 4.3(1.1) nPa when the CAVS is attached to the dynamic expansion system. This corresponds to a lifetime of sensor atoms in their trap of 188(4) s, one of the longest trap lifetimes for an ultra-cold-atom experiment in a room-temperature vacuum environment. The laboratory CAVS includes several features that will allow it to achieve the lowest possible uncertainties and will make possible future studies of systematic effects that could limit its accuracy and operating range. First, the two-chamber design of the laboratory CAVS, separating the atom source from the pressure sensing, eliminates systematic uncertainties related to outgassing from the alkali-metal dispensers. Second, the laboratory CAVS can use either ⁷Li and ⁸⁷Rb as the sensor atom. The former is advantageous for its low fraction of glancing collisions; the latter is perhaps the easiest atom to laser cool. Third, the Bitter-type magnetic coils of the laboratorybased CAVS can generate either a quadrupole or a Ioffe-Pritchard-type magnetic trap, allowing for studies of Majorana loss. Finally, the temperature and number of the sensor atoms can be controlled, allowing for studies of cold atom-cold atom collisions that could limit operation of the CAVS. In principle, the temperature of the vacuum chamber can be changed between 290 K and 305 K leading to a better characterization of the sensor atom loss rate.

We also described our efforts constructing two portable CAVSs, or pCAVSs, based on ⁷Li sensor atoms and designed as potential replacements for ionization gauges, the current *de facto* gauge in the UHV and XHV regimes. We recently used these two pCAVSs to measure the same vacuum. Perhaps not surprisingly for standards, they agree on the measurement of the 41.8 nPa of the vacuum chamber to which they were attached with roughly 3% relative uncertainty. Compared to the laboratory CAVS, the pCAVS sacrifices flexibility for simplicity: the magnetic fields are generated by permanent magnets, the magnetic field gradient for both the MOT and the magnetic trap are the same. The pCAVSs use a novel combined grating MOT/Zeeman slower to cool and trap ⁷Li atoms. At the heart of the devices is a custom grating MOT chip. We described the nano-fabrication steps of these gratings in detail. One of the limiting factors on the accuracy of the pCAVS may be outgassing from the sensor-atom source. We have described two potential replacements.

One of the major ongoing efforts is expanding the theortical calculations of loss rate coefficients L to background gases and sensor atoms other than H_2 and Li. Progress has already been made for ⁷Li+He.^{135,136} In the near future, we also wish to validate the theoretical underpinnings. We need to "compare" the atom loss rate measured by the laboratory CAVS with the known

pressure of specific gas species created by the dynamic expansion system. Equivalently, this measures L of a background gas species which can then be compared to the theoretical value. Further research involves a threeway comparison of the CAVS, pCAVS, and dynamic expansion system. Agreement between all three will yield the strongest experimental validation of the CAVS as a primary vacuum standard.

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CONFLICT OF INTEREST

DSB, JAF, NNK, EBN, JS, and SPE have US Patent 11,291,103. DSB and SPE have filed US Provisional Patent 63/338,047.

DATA AVAILABILITY STATEMENT

Data that support the findings of this study are available upon reasonable request from the authors.

REFERENCES

- ¹R. T. Bayard and D. Alpert, "Extension of the low pressure range of the ionization gauge," Rev. Sci. Instrum. 21, 571-572 (1950)
- ²P. C. Arnold, D. G. Bills, M. D. Borenstein, and S. C. Borichevsky, "Stable and reproducible Bayard-Alpert ionization gauge," J. Vac. Sci. Technol. A 12, 580-586 (1994).
- ³P. A. Redhead, "New hot-filament ionization gauge with low residual current," J. Vac. Sci. Technol. 3, 173-180 (1966).
- ⁴H. Akimichi, T. Tanaka, K. Takeuchi, Y. Tuzi, and I. Arakawa, "Development of a new ionization gauge with Bessel Box type energy analyzer," Vacuum 46, 749-752 (1995).
- ⁵J. A. Fedchak, P. J. Abbott, J. H. Hendricks, P. C. Arnold, and N. T. Peacock, "Review Article: Recommended practice for calibrating vacuum gauges of the ionization type," J. Vac. Sci. Tech. A 36, 030802 (2018)
- ⁶T. G. Brockwell, K. J. Meech, K. Pickens, J. H. Waite, G. Miller, and J. Roberts, "The MAss Spectrometer for Planetary EXploration (MASPEX)," 2016 IEEE Aerospace Conference, 1-17 (2016).
- ⁷G. Dekoulis, *Space Flight* (IntechOpen, 2018) pp. 11–36.
- ⁸R. E. Ellefson, "Methods for in situ QMS calibration for partial pressure and composition analysis," Vacuum 101, 423-432 (2014).
- ⁹E. te Śligte, N. Koster, F. Molkenboer, P. van der Walle, P. Muilwijk, W. Mulckhuyse, B. Oostdijck, C. Hollemans, B. Nijland, P. Kerkhof, M. van Putten, A. Hoogstrate, and A. Deutz,

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accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0120500 "EBL2: high power EUV exposure facility," in *Photomask Technology 2016*, Vol. 9985, edited by B. S. Kasprowicz and P. D. Buck (2016) p. 998520.

¹⁰H. Kibbel and E. Kasper, "Industrial aspects of silicon molecular beam epitaxy," Vacuum **41**, 929–932 (1990).

¹¹J. R. Arthur, "Molecular beam epitaxy," Surf. Sci. **500**, 189–217 (2002).

- ¹²P. W. Palmberg, "Ultrahigh vacuum and surface science," J. Vac. Sci. Technol. A **12**, 946–952 (1994).
- ¹³M. Mozetič, A. Vesel, G. Primc, C. Eisenmenger-Sittner, J. Bauer, A. Eder, G. Schmid, D. Ruzic, Z. Ahmed, D. Barker, K. Douglass, S. Eckel, J. Fedchak, J. Hendricks, N. Klimov, J. Ricker, J. Scherschligt, J. Stone, G. Strouse, I. Capan, M. Buljan, S. Milošević, C. Teichert, S. Cohen, A. Silva, M. Lehocky, P. Humpoliček, C. Rodriguez, J. Hernandez-Montelongo, D. Mercier, M. Manso-Silván, G. Ceccone, A. Galtayries, K. Stana-Kleinschek, I. Petrov, J. Greene, J. Avila, C. Chen, B. Caja-Munoz, H. Yi, A. Boury, S. Lorcy, M. Asensio, J. Bredin, T. Gans, D. O'Connell, J. Brendin, F. Reniers, A. Vincze, M. Anderle, and L. Montelius, "Recent developments in surface science and engineering, thin films, nanoscience, biomaterials, plasma science, and vacuum technology," Thin Solid Films 660, 120–160 (2018).
- ¹⁴H. F. Dylla, "Development of ultrahigh and extreme high vacuum technology for physics research," J. Vac. Sci. Technol. A 21, S25–S33 (2003).
- ¹⁵M. L. Stutzman, P. Adderley, J. Brittian, J. Clark, J. Grames, J. Hansknecht, G. R. Myneni, and M. Poelker, "Characterization of the CEBAF 100 kV DC GaAs photoelectron gun vacuum system," Nucl. Instrum. Methods Phys. Res. A 574, 213–220 (2007).
- ¹⁶K. Jousten, H. Menzer, D. Wandrey, and R. Niepraschk, "New, fully automated, primary standard for generating vacuum pressures between 10^{-10} Pa and 3×10^{-2} Pa with respect to residual pressure," Metrologia **36**, 493–497 (1999).
- ¹⁷K. Jousten, H. Menzer, and R. Niepraschk, "A new fully automated gas flowmeter at the PTB for flow rates between 10⁻¹³ mol/s and 10⁻⁶ mol/s," Metrologia **39**, 519–529 (2002).
- ¹⁸C. R. Tilford, S. Dittmann, and K. E. McCulloh, "The National Bureau of Standards primary high-vacuum standard," J. Vac. Sci. Tech. A 6, 2853–2859 (1988).
- ¹⁹M. Bergoglio and D. Mari, "INRIM continuous expansion system as high vacuum primary standard for gas pressure measurements below 9×10^{-2} Pa," Vacuum 84, 270–273 (2009).
- 20 H. Yoshida, M. Hirata, and H. Akimichi, "Calibration of ultrahigh vacuum gauge from 10^{-9} Pa to 10^{-5} Pa by the two-stage flow-dividing system," Vacuum **86**, 226–231 (2011).
- ²¹D. Li, M. Guo, Y. Cheng, Y. Feng, and D. Zhang, "Vacuumcalibration apparatus with pressure down to 10⁻¹⁰ Pa," J. Vac. Sci. Tech. A **28**, 1099–1104 (2010).
- ²²J. E. Bjorkholm, "Collision-limited lifetimes of atom traps," Phys. Rev. A **38**, 1599–1600 (1988).
- ²³T. Arpornthip, C. A. Sackett, and K. J. Hughes, "Vacuumpressure measurement using a magneto-optical trap," Phys. Rev. A 85, 033420 (2012).
- ²⁴J. Yuan, Z.-H. Ji, Y. Zhao, X.-F. Chang, L. Xiao, and S.-T. Jia, "Simple, reliable, and nondestructive method for the measurement of vacuum pressure without specialized equipment," Applied Optics **52**, 6195 (2013).
- ²⁵R. W. G. Moore, L. A. Lee, E. A. Findlay, L. Torralbo-Campo, G. D. Bruce, and D. Cassettari, "Measurement of vacuum pressure with a magneto-optical trap: A pressure-rise method," Rev. Sci. Instrum. 86, 093108 (2015).
- ²⁶V. B. Makhalov, K. A. Martiyanov, and A. V. Turlapov, "Primary vacuometer based on an ultracold gas in a shallow optical dipole trap," Metrologia 53, 1287–1294 (2016).
- ²⁷ J. L. Booth, P. Shen, R. V. Krems, and K. W. Madison, "Universality of quantum diffractive collisions and the quantum pressure standard," New J. Phys. **21**, 102001 (2019).

- ²⁸P. Shen, K. W. Madison, and J. L. Booth, "Realization of a universal quantum pressure standard," Metrologia 57, 025015 (2020).
- ²⁹P. Shen, K. W. Madison, and J. L. Booth, "Refining the cold atom pressure standard," Metrologia 58, 022101 (2021).
- ³⁰D. E. Pritchard, "Cooling neutral atoms in a magnetic trap for precision spectroscopy," Phys. Rev. Lett. **51**, 1336 (1983).
- ³¹M. O. Mewes, M. R. Andrews, N. J. Van Druten, D. M. Kurn, D. S. Durfee, and W. Ketterle, "Bose-Einstein condensation in a tightly confining dc magnetic trap," Phys. Rev. Lett. **77**, 416 (1996).
- ³²M.-O. Mewes, *Bose-Einstein Condensation of Sodium Atoms*, Ph.D. thesis, Massachusetts Institute of Technology (1997).
- ³³W. Ketterle, D. S. Durfee, and D. M. Stamper-Kurn, "Making, probing and understanding Bose-Einstein condensates," in *Proceedings of the 1998 Enrico Fermi summer school on Bose-Einstein condensation in Varenna, Italy*, edited by M. Inguscio, S. Stringari, and C. E. Wieman (IOS Press, Amsterdam, 1999) pp. 67–176.
- ³⁴E. W. Streed, A. P. Chikkatur, T. L. Gustavson, M. Boyd, Y. Torii, D. Schneble, G. K. Campbell, D. E. Pritchard, and W. Ketterle, "Large atom number Bose-Einstein condensate machines," Rev. Sci. Instrum. **77**, 023106 (2006).
- ³⁵A. L. Migdall, J. V. Prodan, W. D. Phillips, T. H. Bergeman, and H. J. Metcalf, "First observation of magnetically trapped neutral atoms," Phys. Rev. Lett. 54, 2596 (1985).
- ³⁶D. Barker, E. Norrgard, N. Klimov, J. Fedchak, J. Scherschligt, and S. Eckel, "Single-beam Zeeman slower and magneto-optical trap using a nanofabricated grating," Phys. Rev. Applied 11, 064023 (2019).
- ³⁷A. Messiah, *Quantum Mechanics*, 2nd ed. (Dunod, Paris, 1995).
 ³⁸J. J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, 2nd ed. (Addison-Wesley, Boston, 2010).
- ³⁹J. M. V. A. Koelman, S. B. Crampton, H. T. C. Stoof, O. J. Luiten, and B. J. Verhaar, "Spin-exchange frequency shifts in cryogenic and room-temperature hydrogen masers," Phys. Rev. A 38, 3535–3547 (1988).
- ⁴⁰H. T. C. Stoof, J. M. V. A. Koelman, and B. J. Verhaar, "Spinexchange and dipole relaxation rates in atomic hydrogen: Rigorous and simplified calculations," Phys. Rev. B **38**, 4688–4697 (1988).
- ⁴¹C. V. Sukumar and D. M. Brink, "Spin-flip transitions in a magnetic trap," Phys. Rev. A 56, 2451–2454 (1997).
- ⁴²W. Ketterle and N. J. van Druten, "Evaporative cooling of trapped atoms," Adv. At. Mol. Opt. Phys. **37**, 181 (1996).
- ⁴³O. J. Luiten, M. W. Reynolds, and J. T. M. Walraven, "Kinetic theory of the evaporative cooling of a trapped gas," Phys. Rev. A 53, 381–389 (1996).
- ⁴⁴S. Bali, K. M. O'Hara, M. E. Gehm, S. R. Granade, and J. E. Thomas, "Quantum-diffractive background gas collisions in atom-trap heating and loss," Phys. Rev. A **60**, R29–R32 (1999).
- ⁴⁵J. R. Taylor, *Scattering Theory* (Dover Publications, 1972).
- ⁴⁶K. M. O'Hara, S. L. Hemmer, S. R. Granade, M. E. Gehm, J. E. Thomas, V. Venturi, E. Tiesinga, and C. J. Williams, "Measurement of the zero crossing in a Feshbach resonance of fermionic ⁶Li," Phys. Rev. A **66**, 041401 (2002).
- ⁴⁷C. Strauss, T. Takekoshi, F. Lang, K. Winkler, R. Grimm, J. Hecker Denschlag, and E. Tiemann, "Hyperfine, rotational, and vibrational structure of the $a^{3}\Sigma_{u}^{+}$ state of ⁸⁷Rb₂," Phys. Rev. A **82**, 052514 (2010).
- ⁴⁸ J. M. Hutson and C. R. Le Sueur, "molscat: A program for nonreactive quantum scattering calculations on atomic and molecular collisions," Comput. Phys. Commun. **241**, 9–18 (2019), source codes can be found at http://dx.doi.org/10.17632/ rtzgf5mwpn.1.
- ⁴⁹S. Kotochigova, E. Tiesinga, and P. S. Julienne, "Relativistic ab initio treatment of the second-order spin-orbit splitting of the $a^{3}\Sigma_{u}^{+}$ potential of rubidium and cesium dimers," Phys. Rev. A **63**, 012517 (2000).

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the author's peer reviewed,

- accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset

 - PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0120500

- ⁵⁰J. M. Gerton, C. A. Sackett, B. J. Frew, and R. G. Hulet, "Dipolar relaxation collisions in magnetically trapped ⁷Li," Phys. Rev. A **59**, 1514–1516 (1999).
- ⁵¹C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, "Feshbach resonances in ultracold gases," Rev. Mod. Phys. 82, 1225-1286 (2010).
- ⁵²S. E. Pollack, D. Dries, and R. G. Hulet, "Universality in threeand four-body bound states of ultracold atoms," Science 326, 1683-1685 (2009).
- ⁵³P. Dyke, S. E. Pollack, and R. G. Hulet, "Finite-range corrections near a Feshbach resonance and their role in the efimov effect," Phys. Rev. A 88, 023625 (2013).
- ⁵⁴E. A. Burt, R. W. Ghrist, C. J. Myatt, M. J. Holland, E. A. Cornell, and C. E. Wieman, "Coherence, correlations, and collisions: What one learns about Bose-Einstein condensates from their decay," Phys. Rev. Lett. 79, 337-340 (1997).
- ⁵⁵M. S. Child, *Molecular collision theory* (Academic Press, New York, 1974).
- ⁵⁶C. Makrides, D. S. Barker, J. A. Fedchak, J. Scherschligt, S. Eckel, and E. Tiesinga, "Elastic rate coefficients for Li+H₂ collisions in the calibration of a cold-atom vacuum standard,' Phys. Rev. A 99, 042704 (2019).
- $^{57}\mathrm{B.}$ Gao, "Solutions of the Schrödinger equation for an attractive $1/r^6$ potential," Phys. Rev. A 58, 1728–1734 (1998).
- $^{58}\mathrm{B.}$ Gao, "Analytic description of atomic interaction at ultracold temperatures: The case of a single channel," Phys. Rev. A 80, 012702 (2009)
- ⁵⁹S. Bovino, M. Wernli, and F. A. Gianturco, "Fast LiH destruction in reaction with H: Quantum calculations and astrophysical consequences," ApJ 699, 383-387 (2009).
- ⁶⁰C. Makrides, D. S. Barker, J. A. Fedchak, J. Scherschligt, S. Eckel, and E. Tiesinga, "Erratum: Elastic rate coefficients for Li+H₂ collisions in the calibration of a cold-atom vacuum standard [Phys. Rev. A 99, 042704 (2019)]," Phys. Rev. A 105, 039903 (2022).
- ⁶¹M. Li and H. F. Dylla, "Model for the outgassing of water from metal surfaces," J. Vac. Sci. Technol. A 11, 1702–1707 (1993).
- ⁶²J. A. Fedchak, J. K. Scherschligt, S. Avdiaj, D. S. Barker, S. P. Eckel, B. Bowers, S. O'Connell, and P. Henderson, "Outgassing rate comparison of seven geometrically similar vacuum chambers of different materials and heat treatments," J. Vac. Sci. Technol. B 39, 24201 (2021).
- ⁶³M. Sefa, J. A. Fedchak, and J. Scherschligt, "Investigations of medium-temperature heat treatments to achieve low outgassing rates in stainless steel ultrahigh vacuum chambers," J. Vac. Sci. Technol. A 35, 041601 (2017).
- ⁶⁴M. A. A. Mamun, A. A. Elmustafa, M. L. Stutzman, P. A. Adderley, and M. Poelker, "Effect of heat treatments and coatings on the outgassing rate of stainless steel chambers," J. Vac. Sci. Technol. A 32, 021604 (2014).
- $^{65}\mathrm{D.}$ Grant, D. Cummings, and D. Blackburn, "Hydrogen in 316 steel — diffusion, permeation and surface reaction," J. Nucl. Mater. 152, 139–145 (1988).
- ⁶⁶J. A. Fedchak, J. Scherschligt, D. Barker, S. Eckel, A. P. Farrell, and M. Sefa, "Vacuum furnace for degassing stainless-steel vacuum components," Journal of Vacuum Science & Technology A 36, 023201 (2018), https://doi.org/10.1116/1.5016181.
- ⁶⁷L. Westerberg, B. Hjörvarsson, E. Wallén, and A. Mathewson, "Hydrogen content and outgassing of air-baked and vacuumfired stainless steel," Vacuum 48, 771-773 (1997).
- ⁶⁸C. D. Park, S. M. Chung, X. Liu, and Y. Li, "Reduction in hydrogen outgassing from stainless steels by a mediumtemperature heat treatment," J. Vac. Sci. Technol. A 26, 1166-1171 (2008).
- ⁶⁹K. Battes, C. Day, and V. Hauer, "Outgassing rate measurements of stainless steel and polymers using the difference method," J. Vac. Sci. Technol. A 33, 021603 (2015).
- $^{70}\mathrm{M}.$ Zucker, "The LIGO 4 km vacuum system: Design, construction, features and faults," (Presentation for NSF Workshop on Large UHV Systems for Frontier Scientific Research, LIGO Liv-

ingston, 2019, 2019).

- ⁷¹M. Knudsen, "Die Gesetze der Molekularströmung und der inneren Reibungsströmung der Gase durch Röhren," Ann. Phys. **333**, 75–130 (1909).
- $^{72}\mathrm{M.}$ Knudsen, "Die Molekularströmung der Gase durch Offnungen und die Effusion," Ann. Phys. 333, 999-1016 (1909).
- ⁷³P. Clausing, "Über die Strömung sehr verdünnter Gase durch Röhren von beliebiger Länge," Ann. Phys. 404, 961-989 (1932).
- ⁷⁴A. S. Berman, "Free molecule transmission probabilities," J. App. Phys. 36, 3356–3356 (1965).
- ⁷⁵D. van Essen and W. C. Heerens, "On the transmission probability for molecular gas flow through a tube," J. Vac. Sci. Technol. **13**, 1183–1187 (1976).
- ⁷⁶K. E. McCulloh, C. R. Tilford, C. D. Ehrlich, and F. G. Long, "Low-range flowmeters for use with vacuum and leak standards," J. Vac. Sci. Technol. A 5, 376-381 (1987).
- $^{77}\mathrm{J.\,E.}$ van den Berg, S. H. Turkesteen, E. B. Prinsen, and S. Hoekstra, "Deceleration and trapping of heavy diatomic molecules using a ring-decelerator," Eur. Phys. J. D 66, 235 (2012).
- ⁷⁸K. Jousten, G. Messer, and D. Wandrey, "A precision gas flowmeter for vacuum metrology," Vacuum 44, 135–141 (1993).
- ⁷⁹H. Yoshida, K. Arai, H. Akimichi, and T. Kobata, "Newly developed standard conductance element for in situ calibration of high vacuum gauges," Measurement 45, 2452–2455 (2012).
- ⁸⁰J. Scherschligt, D. Barker, S. Eckel, J. Fedchak, and E. Newsome, "Stability of bakeable capacitance diaphragm gauges," Vacuum **197**, 110801 (2022).
- ⁸¹S. Eckel, D. S. Barker, J. Fedchak, E. Newsome, J. Scherschligt, and R. Vest, "A constant pressure flowmeter for extreme-high vacuum," Metrologia 59, 045014 (2022).
- 82 In principle, we could choose any position of the piston for $\Delta V_{\text{piston}} = 0, \ e.g.$ fully retracted.
- ⁸³The identification of commercial products is for information only and does not imply recommendation or endorsement by the National Institute of Standards and Technology.
- ⁸⁴J. Ricker, J. Hendricks, T. Bock, D. Pražák, T. Kobata, J. Torres, I. Sadkovskaya, P. Dominik, T. Kobata, J. Torres, and I. Sadkovskava, "Final report on the key comparison CCM.P-K4.2012 in absolute pressure from 1 Pa to 10 kPa," Metrologia **54**, 1–37 (2017).
- ⁸⁵S. Dushman and J. Lafferty, Scientific Foundations of Vacuum Technique (John Wiley and Sons, Inc., 2018) pp. 82–87.
- ⁸⁶W. D. Phillips and H. Metcalf, "Laser deceleration of an atomic beam," Phys. Rev. Lett. 48, 596-599 (1982).
- ⁸⁷E. L. Raab, M. Prentiss, A. Cable, S. Chu, and D. E. Pritchard, "Trapping of neutral sodium atoms with radiation pressure," Phys. Rev. Lett. 59, 2631-2634 (1987).
- ⁸⁸H. Metcalf and P. van der Straten, Laser Cooling and Trapping (Springer-Verlag New York Inc., New York, 1999).
- ⁸⁹C. Foot, Atomic Physics (Oxford University Press Inc., New York, 2005).
- ⁹⁰J. Scherschligt, J. A. Fedchak, D. S. Barker, S. Eckel, N. Klimov, C. Makrides, and E. Tiesinga, "Development of a new UHV/XHV pressure standard (cold atom vacuum standard)," Metrologia 54, S125 (2017).
- ⁹¹S. Eckel, D. S. Barker, J. A. Fedchak, N. N. Klimov, E. Norrgard, J. Scherschligt, C. Makrides, and E. Tiesinga, "Challenges to miniaturizing cold atom technology for deployable vacuum metrology," Metrologia 55, S182 (2018).
- ⁹²D. O. Sabulsky, C. V. Parker, N. D. Gemelke, and C. Chin, "Efficient continuous-duty Bitter-type electromagnets for cold atom experiments," Rev. Sci. Instrum. 84, 104706 (2013).
- ⁹³T. Luan, T. Zhou, X. Chen, and Z. Ma, "A modified Bitter-type electromagnet and control system for cold atom experiments," Rev. Sci. Instrum. 85, 024701 (2014).
- ⁹⁴Y. Long, F. Xiong, V. Gaire, C. Caligan, and C. V. Parker, "Alloptical production of ⁶Li molecular Bose-Einstein condensates in excited hyperfine levels," Phys. Rev. A 98, 043626 (2018).
- ⁹⁵J. L. Siegel, D. S. Barker, J. A. Fedchak, J. Scherschligt, and S. Eckel, "A Bitter-type electromagnet for complex atomic trap-

accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0120500

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the author's peer reviewed,

- ping and manipulation," Rev. Sci. Instrum. 92, 033201 (2021).
 ⁹⁶T. G. Tiecke, S. D. Gensemer, A. Ludewig, and J. T. M. Walraven, "High-flux two-dimensional magneto-optical-trap source for cold lithium atoms," Phys. Rev. A 80, 013409 (2009).
 ⁹⁷K. Wright, private communication (2017).
- ⁹⁸N. F. Ramsey, *Molecular Beams* (Oxford University Press, London, 1956).
- ⁹⁹A. R. Perry, An Apparatus for Light-less Artificial Gauge Fields and New Imaging Techniques, Ph.D. thesis, University of Maryland (2015).
- ¹⁰⁰Z. S. Smith, D. S. Barker, and A. Restelli, "Bipolar MOSFET current servo for shim/trim coils," (2019), source code can be found at https://github.com/JQIamo/bipolar-mosfet-board.
- 101 Note that this equation is different from Eq. (1) in Ref. 95 due to a 45° rotation about +z to bring the two coordinate systems into alignment.
- ¹⁰²F. Bitter, "The Design of Powerful Electromagnets Part II. The Magnetizing Coil," Rev. Sci. Instrum. 7, 482 (1936).
- ¹⁰³L. Ricci, L. M. Martini, M. Franchi, and A. Bertoldi, "A currentcarrying coil design with improved liquid cooling arrangement," Rev. Sci. Instrum. 84, 065115 (2013).
- ¹⁰⁴N. McKay Parry, M. Baker, T. Neely, T. Carey, T. Bell, and H. Rubinsztein-Dunlop, "Note: High turn density magnetic coils with improved low pressure water cooling for use in atom optics," Rev. Sci. Instrum. 85, 086103 (2014).
- ¹⁰⁵K. Roux, B. Cilenti, V. Helson, H. Konishi, and J.-P. Brantut, "Compact bulk-machined electromagnets for quantum gas experiments," SciPost Physics 6, 048 (2019).
- ¹⁰⁶We cannot determine whether the coordinate systems defined by the curvature and anti-bias coil pairs are rotated with respect to each other. However, this seems unlikely because both coil pairs are mounted to the same water distribution manifold.
- ¹⁰⁷O. Chubar, P. Elleaume, and J. Chavanne, "A three-dimensional magnetostatics computer code for insertion devices," J. Synchrotron Rad. 5, 481 (1998).
- ¹⁰⁸M. O. Mewes, G. Ferrari, F. Schreck, A. Sinatra, and C. Salomon, "Simultaneous magneto-optical trapping of two lithium isotopes," Phys. Rev. A **61**, 011403(R) (1999).
- ¹⁰⁹A. T. Grier, I. Ferrier-Barbut, B. S. Rem, M. Delehaye, L. Khaykovich, F. Chevy, and C. Salomon, "A-enhanced sub-Doppler cooling of lithium atoms in D₁ gray molasses," Phys. Rev. A 87, 063411 (2013).
- ¹¹⁰A. Burchianti, G. Valtolina, J. A. Seman, E. Pace, M. De Pas, M. Inguscio, M. Zaccanti, and G. Roati, "Efficient all-optical production of large ⁶Li quantum gases using D₁ gray-molasses cooling," Phys. Rev. A **90**, 043408 (2014).
- ¹¹¹P. D. Lett, R. N. Watts, C. I. Westbrook, W. D. Phillips, P. L. Gould, and H. J. Metcalf, "Observation of atoms laser cooled below the doppler limit," Phys. Rev. Lett. **61**, 169–172 (1988).
- ¹¹²C. Valentin, M. C. Gagné, J. Yu, and P. Pillet, "One-dimension sub-doppler molasses in the presence of static magnetic field," EPL **17**, 133 (1992).
- ¹¹³G. Grynberg and J.-Y. Courtois, "Proposal for a magnetooptical lattice for trapping atoms in nearly-dark states," EPL 27, 41 (1994).
- ¹¹⁴D. Boiron, C. Triché, D. R. Meacher, P. Verkerk, and G. Grynberg, "Three-dimensional cooling of cesium atoms in four-beam gray optical molasses," Phys. Rev. A **52**, R3425 (1995).
- ¹¹⁵M. S. Shahriar, P. R. Hemmer, M. G. Prentiss, P. Marte, J. Mervis, D. P. Katz, N. P. Bigelow, and T. Cai, "Continuous polarization-gradient precooling-assisted velocity-selective coherent population trapping," Phys. Rev. A 48, R4035 (1993).
- ¹¹⁶P. Marte, R. Dum, R. Taïeb, P. Zoller, M. S. Shahriar, and M. Prentiss, "Polarization-gradient-assisted subrecoil cooling: Quantum calculations in one dimension," Phys. Rev. A 49, 4826 (1994).
- ¹¹⁷M. Weidemüller, T. Esslinger, M. A. Ol'shanii, A. Hemmerich, and T. W. Hänsch, "A novel scheme for efficient cooling below

the photon recoil limit," EPL **27**, 109 (1994).

- ¹¹⁸D. R. Fernandes, F. Sievers, N. Kretzschmar, S. Wu, C. Salomon, and F. Chevy, "Sub-Doppler laser cooling of fermionic ⁴⁰K atoms in three-dimensional gray optical molasses," EPL **100**, 63001 (2012).
- ¹¹⁹P. D. Lett, W. D. Phillips, S. L. Rolston, C. E. Tanner, R. N. Watts, and C. I. Westbrook, "Optical molasses," J. Opt. Soc. Am. B 6, 2084 (1989).
- ¹²⁰A. Kastler, "Quelques suggestions concernant la production optique et la détection optique dune inégalité de population des niveaux de quantifigation spatiale des atomes. application à lexpérience de stern et gerlach et à la résonance magnétique," Journal de Physique et le Radium 11, 255 (1950).
- ¹²¹J. R. Ensher, The First Experiments with Bose-Einstein Condensation of ⁸⁷Rb, Ph.D. thesis, University of Colorado (1998).
- ¹²²C. D. Herold, Ultracold Mixtures of Rubidium and Ytterbium for Open Quantum System Engineering, Ph.D. thesis, University of Maryland, College Park (2014).
- ¹²³This red detuning is limited by our laser system, which uses acousto-optic modulators to realize small frequency shifts.
- ¹²⁴D. Barker, N. Klimov, E. Tiesinga, J. Fedchak, J. Scherschligt, and S. Eckel, "Progress towards comparison of quantum and classical vacuum standards," Meas. Sensors 18, 100229 (2021).
- 125 With only 10⁵ atoms, we are unable to accurately measure the temperature and thus assume the initial temperature is set by the RF knife.
- ¹²⁶L. H. Ehinger, B. P. Acharya, D. S. Barker, J. A. Fedchak, J. Scherschligt, E. Tiesinga, and S. Eckel, "Comparison of two multiplexed portable cold-atom vacuum standards," AVS Quantum Science 4, 034403 (2022).
- ¹²⁷D. S. Barker, E. B. Norrgard, N. N. Klimov, J. A. Fedchak, J. Scherschligt, and S. Eckel, "Λ-Enhanced Gray Molasses in a Tetrahedral Laser Beam Geometry," Opt. Express **30**, 9959 (2022).
- ¹²⁸J. P. McGilligan, P. F. Griffin, E. Riis, and A. S. Arnold, "Diffraction-grating characterization for cold-atom experiments," J. Opt. Soc. Am. B **33**, 1271 (2016).
- ¹²⁹E. Hecht, *Optics*, Pearson education (Addison-Wesley, 2002).
- ¹³⁰W. Kern and D. A. Puotinen, "Cleaning solutions based on hydrogen peroxide for use in silicon semiconductor technology," RCA Rev. **31**, 187 (1970).
- ¹³¹M. A. Gosálvez, "Chapter ten manufacture and processing of mems structures," in *Handbook of Silicon Based MEMS Materials and Technologies*, Micro and Nano Technologies, edited by V. Lindroos, M. Tilli, A. Lehto, and T. Motooka (William Andrew Publishing, Boston, 2010) pp. 157–177.
- ¹³²E. B. Norrgard, D. S. Barker, J. A. Fedchak, N. Klimov, J. Scherschligt, and S. Eckel, "Note: A 3D-printed alkali metal dispenser," Rev. Sci. Instrum. 89, 056101 (2018).
- ¹³³D. S. Barker, E. B. Norrgard, J. Scherschligt, J. A. Fedchak, and S. Eckel, "Light-induced atomic desorption of lithium," Phys. Rev. A **98**, 043412 (2018).
- ¹³⁴C. Klempt, T. van Zoest, T. Henninger, O. Topic, E. Rasel, W. Ertmer, and J. Arlt, "Ultraviolet light-induced atom desorption for large rubidium and potassium magneto-optical traps," Phys. Rev. A **73**, 013410 (2006).
- ¹³⁵C. Makrides, D. S. Barker, J. A. Fedchak, J. Scherschligt, S. Eckel, and E. Tiesinga, "Collisions of room-temperature helium with ultracold lithium and the van der Waals bound state of HeLi," Phys. Rev. A **101**, 012702 (2020).
- ¹³⁶C. Makrides, D. S. Barker, J. A. Fedchak, J. Scherschligt, S. Eckel, and E. Tiesinga, "Erratum: Collisions of roomtemperature helium with ultracold lithium and the van der Waals bound state of HeLi [Phys. Rev. A **101**, 012702 (2020)]," Phys. Rev. A **105**, 029902 (2022).















































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