

# **Optical Lattice Clock with Spin-1/2 Ytterbium Atoms**

by

**N. D. Lemke**

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written by N. D. Lemke  
has been approved for the Department of Physics

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Dr. Jun Ye

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Dr. Chris Oates

Date \_\_\_\_\_

The final copy of this thesis has been examined by the signatories, and we find that both the content and the form meet acceptable presentation standards of scholarly work in the above mentioned discipline.

Lemke, N. D. (Ph.D., Physics)

Optical Lattice Clock with Spin-1/2 Ytterbium Atoms

Thesis directed by Dr. Jun Ye

An optical lattice clock probes a spectrally narrow electronic transition in an ensemble of optically trapped, laser-cooled atoms, for use as a time and frequency standard. To date, several lattice clocks have been demonstrated with superior stability and accuracy compared to primary frequency standards based on microwave transitions. Yet, the question of which atomic system (including the element and isotope) performs best as a lattice clock remains unsettled. This thesis describes the first detailed investigation of an optical lattice clock using a spin-1/2 isotope of the ytterbium atom. A spin-1/2 system possesses several advantages over higher-spin systems, including a simplified level structure (allowing for straightforward manipulation of the nuclear spin state) and the absence of any tensor light shift from the confining optical lattice. Moreover, the ytterbium atom (Yb) stands among the leading lattice clock candidates, offering a high-performance optical clock with some degree of experimental simplicity. The frequency stability of the Yb clock is highlighted by resolving an ultra-narrow clock spectrum with a full-width at half-maximum of 1 Hz, corresponding to a record quality factor  $Q = \nu_0/\Delta\nu = 5 \times 10^{14}$ . Moreover, this system can be highly accurate, which is demonstrated by characterizing the Yb clock frequency at the  $3 \times 10^{-16}$  level of fractional uncertainty, with further progress toward a ten-fold improvement also presented. To reach this low level of uncertainty required careful consideration of important systematic errors, including the identification of the Stark-canceling wavelength, where the clock's sensitivity to the lattice intensity is minimized, a precise determination of the static polarizability of the clock transition, and the measurement and control of atom-atom collisions.

## Dedication

To my family.



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## Chapter 1

### Introduction

This thesis details the first experimental investigation of an optical lattice clock using an isotope with nuclear spin  $I = 1/2$ . While lattice clocks based on atoms with higher nuclear spin [1] and with no nuclear spin [2] have been demonstrated, here we highlight a few special properties of a spin-1/2 system. To set the stage for this discussion, we will first review some basic principles of atomic clocks, followed by a brief discussion of several applications that call for higher-performing atomic clocks. Then, in Sec. 1.4, we will examine why a spin-1/2 system may be the best choice for state-of-the-art timekeeping with an optical lattice clock.

#### 1.1 Atomic clocks

Since 1967, the unit of time in the International System of Units (SI) has been defined in terms of the energy difference between the two lowest states of cesium atoms [3, 4]<sup>1</sup>. This definition is realized in the laboratory by steering a microwave oscillator to stay resonant with the Cs atoms while simultaneously counting the number of oscillations (“ticks”) that have passed. Atomic transitions are ideally suited for timekeeping because the atom’s energy levels are largely immune to environmental effects. Because microwave radiation oscillates very quickly (about 10 billion times per second), each cycle is short in time, allowing for highly precise measurements of time and frequency. Today’s Cs primary frequency standards are extremely accurate, with uncertainty at just a few parts in  $10^{16}$  [5, 6, 7, 8, 9, 10]. This is equivalent to saying that the clock

---

<sup>1</sup> Specifically, the definition of the second is “the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium-133 atom” [3].

would neither gain nor lose one second in 100 million years.

This exceptional accuracy is made possible by the stability, or precision, of atomic clocks. Two figures of merit that largely determine the stability of the clock are its resonance quality factor ( $Q = \nu_0/\Delta\nu$ ) and its measurement signal-to-noise ratio (S/N). The quality factor is a dimensionless quantity that gives the width of a resonance,  $\Delta\nu$ , in comparison to its center frequency,  $\nu_0$ . For the best Cs clocks, a linewidth of 1 Hz results in  $Q = 10^{10}$ . The S/N is also dimensionless, and it gives information about the fidelity of each measurement. In general, there are many sources of noise that could diminish this quantity, but under certain conditions it is possible to reach the “standard quantum limit” of  $S/N = \sqrt{N_{atom}}$  with  $N_{atom}$  the number of atoms interrogated. For a typical value of  $10^6$  atoms, the S/N is 1000. The product of  $Q$  and S/N gives the fractional precision (here,  $10^{13}$ ), which is indeed not far from the typical stability of Cs fountain clocks [5, 9]. This means that after just one measurement (lasting approximately 1 second), the frequency has already been found to 13 digits, and subsequent measurements strung together will continue to increase the combined precision. With this level of stability, it is possible to quickly and thoroughly evaluate possible sources of systematic error and to compare two clocks to see how well they agree.

To achieve this level of inaccuracy has taken more than 50 years of scientific and technical advances. One very important step along the way was the advent of laser cooling of atoms [11, 12] and its application to atomic clocks [13, 14]. The key advantage to cold atoms lies in their slowed velocity, which results in longer interaction times and reduced Doppler shifts. State-of-the-art microwave clocks typically use a fountain geometry, in which a ball of laser-cooled atoms is tossed straight up before falling back under gravity. This atomic fountain, which is very successful at canceling Doppler effects [15], is made possible by the ultracold atomic temperature.

So what limits the accuracy of cold-atom microwave fountain clocks such as NIST-F1? The full answer includes a long list of systematic effects, each of which needs to be evaluated to smaller and smaller levels of uncertainty. But with a fixed  $Q$  and a clock stability approaching its fundamental limit, smaller uncertainties require longer averaging times, and eventually this becomes impractical or even impossible. For this reason, it is interesting to consider atomic systems with

potentially higher stability, which in turn offers the possibility for a corresponding reduction in absolute uncertainty.

## 1.2 Optical clocks and the optical frequency comb

The clearest path for developing a higher stability clock is to use a higher frequency transition. Optical transitions (so-called because they absorb and emit light visible to human eyes) have frequencies in the hundreds of terahertz range, or nearly 100 000 times higher than microwave clocks. These optical clocks thus offer tremendous advantages for improved time and frequency metrology, and sometime (perhaps in the next 10 years) the SI second will be redefined in terms of an optical clock transition.

In the past, one disadvantage to optical frequency standards was the lack of an optical clockwork — a way of counting the ticks [16, 17, 18, 19, 20]. Because optical frequencies are so high ( $10^{15}$  oscillations per second), standard electronic counters cannot be used. Around the year 2000, this problem was solved by the development of the optical frequency comb, for which a portion of the 2005 Nobel Prize in physics was awarded [21, 22, 23, 24, 25, 26, 27, 28]. The optical frequency comb is a pulsed laser that outputs very short pulses of light. Each pulse is composed of thousands of laser modes that form a grid (or a “comb”) in frequency space, much like the fine tick marks on a ruler that allow for precise length measurements (see Fig. 1.1(a)). These optical frequency combs are useful both for comparing two optical clocks at different frequencies and for dividing an optical signal to the microwave domain where it can be counted, and they have enabled vast progress in the field of optical frequency metrology over the last decade. We will consider the comb in slightly more detail in Ch. 7.

The basic scheme of an optical clock is shown in Fig 1.1(b). A laser is electronically stabilized to a high-finesse optical cavity, and the cavity-locked laser comprises the clock’s oscillator (typically called the local oscillator, or LO). The optical cavity is designed to have a very constant length (i.e., the distance between the two reflecting mirrors), as the length stability of the cavity directly determines the frequency stability of the laser. While the optical cavity provides an excellent means

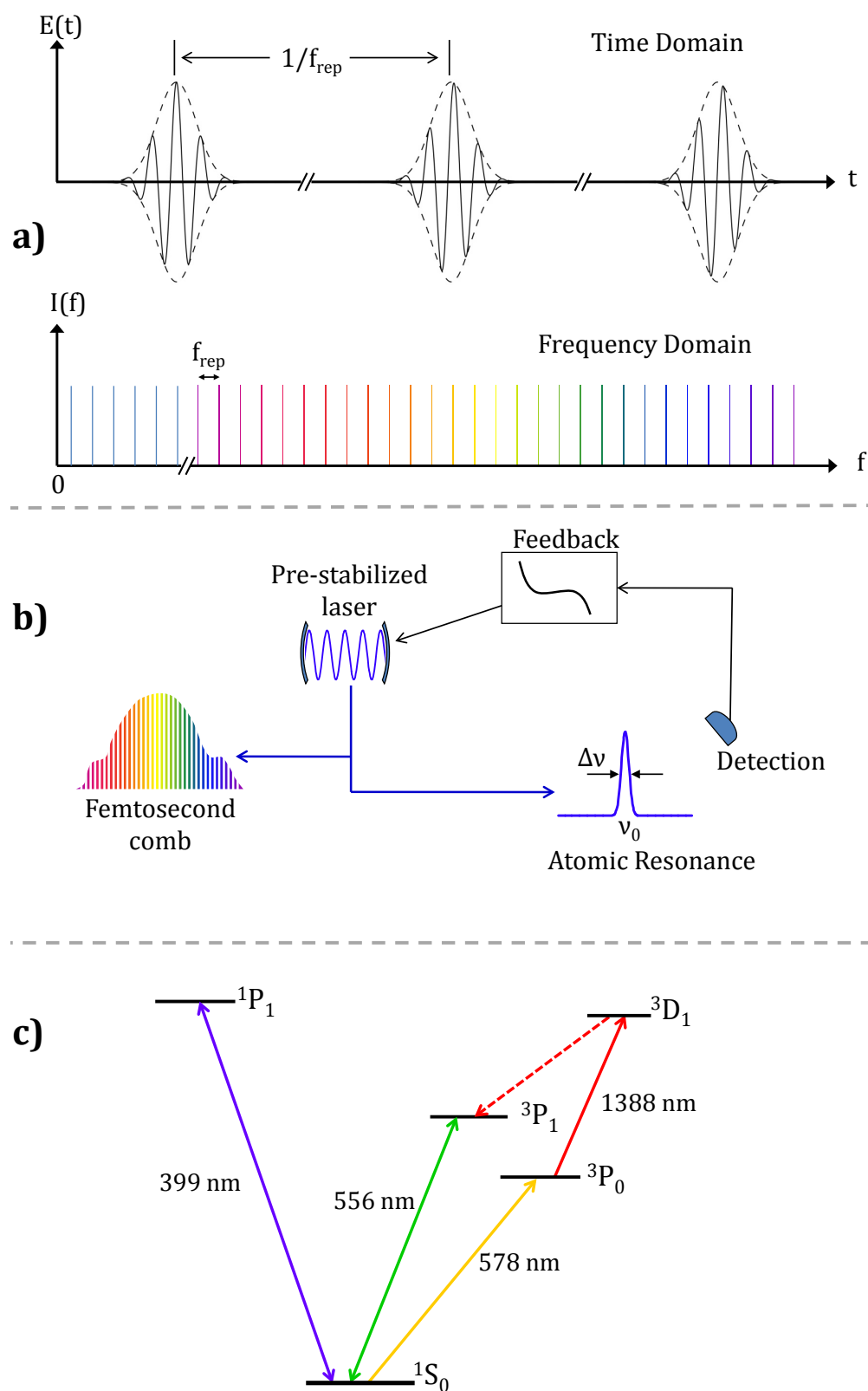


Figure 1.1: a) Time- and frequency-domain depiction of the frequency comb output. b) Block diagram of an optical clock. c) Relevant energy levels in Yb.

for reducing the noise of the laser, it does not provide a good long-term reference (nor is its length a fundamental physical quantity with which to form a universal standard), so an atomic system serves as the long-term frequency reference. Specifically, light from the cavity-stabilized laser probes an optical transition in the atomic system, and electronic corrections are applied to the laser frequency to hold it on resonance with the atom(s). The final component in the optical clock scheme is the optical frequency comb, as mentioned above, which acts as a frequency counter by accumulating trillions of oscillations on the optical signal before outputting a “tick”.

Two competing technologies for the atomic reference are currently being pursued at metrology labs throughout the world: trapped-ion clocks and optical lattice clocks [29, 30]. While there are a number of factors that will play into the ultimate decision of which atomic system becomes the new standard, not to mention which system(s) will perform best as a portable device for commercial and space applications, it is likely that both types will find useful applications. Let us first examine the potential stability of these systems. Trapped-ion clocks typically interrogate one electrically-charged atom, confined by RF electromagnetic fields and cooled to its motional ground state [31, 32, 33, 34, 35, 36, 37]. These ion clocks have thus far been limited to one clock atom because of the possible clock errors due to Coulomb repulsion between multiple atoms. For a single-trapped-ion clock, atomic spectra of few-hertz width [38, 39] and a S/N of 1 yield a fractional precision of  $10^{14}$  in a single measurement.

Optical lattice clocks, by contrast, interrogate an ensemble of laser-cooled atoms confined in an optical potential [40, 41, 42, 1, 43]. This optical potential is formed by a standing-wave laser field known as an optical lattice and is tuned to a specific wavelength (the “magic wavelength”) where it does not perturb the clock frequency [40, 44]. Just as with ion clocks, the resonances in lattice clocks can be very narrow, leading to similar  $Q$ -factors of  $10^{14}$  or higher [45, 43, 46]. But, here the large number of quantum absorbers results in a S/N of 100 to 1000, leading to a potential precision exceeding  $10^{17}$ . From these considerations, we can see the optical lattice clocks have the potential for 10,000-fold improvement in stability over microwave clocks. Moreover, as we will see later in this thesis, these systems also possess the potential to be highly accurate, making them excellent

candidates for state-of-the-art metrology. However, we also note that many of these gains have yet to be realized. Due to technical noise sources, the stability of lattice clocks has not reached the level mentioned above, but is instead similar to that of the ion clocks [47, 1, 48, 46]. Moreover, the best accuracy demonstrated so far [1, 49, 43, 50] is only slightly better than that of the best microwave clocks, and significantly worse than that of the best ion clocks [36, 37]. So while these lattice clock systems remain tantalizing, there are still many significant obstacles to overcome. In this thesis, we will examine some of these obstacles and demonstrate some new techniques to overcome them.

### 1.3 Applications for ultra-precise clocks

Many of today’s technologies in communications and navigation (notably GPS) have been enabled by atomic clocks, and it is expected that the vast improvements in timekeeping offered by optical clocks will further enable new technologies. While it is impossible to fully predict what scientific and technological impact optical clocks will ultimately have, we can already list some known applications for these higher-performing clocks. Following are a few of the most significant.

#### i) Variation of constants

The search for time-variation in the fundamental constants is an active field of research in which atomic clocks are just one piece, albeit an important one. There are several reasons to search for such variations, ranging from tests of new cosmological and unification theories to explanations for the “fine-tuning” question of why the current values of fundamental constants are capable of supporting life on earth [51, 52, 53]. While astronomical data are useful for assessing the values of fundamental constants in the distant past, laboratory searches offer precise measurements of the current drift rates in a highly controlled setting. Unlike microwave transitions, which are primarily sensitive to changes in the electron-proton mass ratio ( $\mu = m_e/m_p$ ), optical transitions are primarily sensitive to changes in the fine structure constant,  $\alpha = e^2/(4\pi\epsilon_0\hbar c)$  [54, 55]. In fact, the tightest constraint to date on  $\dot{\alpha}$  was set by the  $\text{Al}^+$  and  $\text{Hg}^+$  optical clocks at NIST [36]. Fractional changes in the clock transition frequency are



related to changes in  $\alpha$  by

$$\frac{\delta\nu}{\nu} = K \frac{\delta\alpha}{\alpha} \quad (1.1)$$

where  $K$  depends on the atomic structure. Generally, lattice clocks do not have especially high sensitivities ( $K_{\text{Sr}} = 0.06$ ,  $K_{\text{Yb}} = 0.32$ ,  $K_{\text{Hg}^+} = -2.94$ ) so they may be most useful in this regard by serving as “anchor” lines against which atomic systems with higher sensitivity may be compared [56]. In the same manner, the Sr lattice clock transition, which has been compared to the Cs microwave transition in several labs throughout the world, served as a stable reference for constraining  $\dot{\mu}$  in Cs [55].

ii) Testing relativity and the equivalence principle

Local position invariance (LPI), which is a consequence of Einstein’s equivalence principle [57, 58], requires that the outcome of a non-gravitational measurement does not depend on the value of the local gravitational potential. Space-born optical clocks could test this by measuring the frequency ratio of two clocks of different species on a satellite and comparing it to the value measured on earth. Alternatively, the ratio could be monitored as the satellite traverses a highly eccentric orbit, thus modulating the gravitational potential in time. In this case the constraints on the two clocks’ accuracies are reduced, though their medium-term (few hour) stability must be quite good. These techniques are expected to improve upon the best measurement of LPI by more than 5 orders of magnitude [59, 60].

Similarly, the absolute gravitational redshift could be measured with space-based clocks, either with two clocks on different circular orbits, or with one clock in a highly-eccentric orbit and one stationary [59]. Here the expected improvement from previous results is four orders [60]. Additionally, with a reference clock in space, earth’s gravitational field could be measured with greater accuracy, enabling an improved mapping of the geoid [61].

Some unification theories predict that the values of fundamental constants are coupled to the gravitational field, which would violate LPI. While this could be explored most neatly with a deep space mission, it could also be observable on earth due to the ellipticity of earth’s orbit.

Any absence of change in the clock frequency, over the timescale of earth's orbital period, constrains the possible size of these couplings [55].

iii) Low noise microwave generation

Photodetection of a femtosecond frequency comb, referenced to an optical clock, yields an electronic signal at a harmonic of the repetition rate (typically chosen near 10 GHz) with exceptionally low phase noise. While there are additional noise sources that can play a role, these are tractable, and microwave signals whose noise properties are nearly as good as those of the optical clock have been produced [62, 63]. The technical applications calling for these low phase noise microwaves include the following: remote synchronization of large scientific facilities such as synchrotron and accelerators [64, 65]; the local oscillator in a microwave clock [66]; and very-long baseline interferometry (VLBI), in which signals at spatially separate radio telescopes can be combined (with the help of a fine timing system) to yield exceptional angular resolution in studying astrophysical phenomena [67].

iv) Realization of SI units

As mentioned above, the SI second is defined by a transition in atomic cesium, requiring Cs atomic clocks to realize the definition. While some optical clocks have already demonstrated superior repeatability compared to the best microwave clocks, they cannot, by definition, be accurate. For this reason, the definition of the SI second will almost certainly be changed someday to an optical transition, which will then require metrology labs the world over to build new atomic clocks based on the particular optical transition selected.

With the speed of light defined to be exactly  $c = 299\,792\,458$  m/s, the meter is then defined as the distance light travels (in vacuum) in a time of  $1/c \approx 3$  ns [68]. This definition can only be realized accurately with a Cs atomic clock, which defines the second, together with an optical frequency comb that links visible laser light with the microwave clock. However, some optical transitions, including those of  $\text{Hg}^+$  ion and Sr lattice, have been recognized as secondary representations of the SI second, which means they also can be used for realizing

the SI meter. The accuracy gained by defining the second by an optical transition could, at least in principle, lead to more accurate length measurements as well. With better measures of the fine structure and Rydberg constants, it may be possible to someday realize other physical quantities (like mass) with optical atomic clocks [69].

## 1.4 Spin-1/2 ytterbium atoms

The first proposal for an optical lattice clock called for spectroscopy of a narrow optical transition in ultracold strontium atoms [40]. Since then, experimental groups have begun researching not only strontium (Sr) [70, 71, 72, 73, 74], but also ytterbium (Yb) [75, 76, 77, 78, 79] and mercury (Hg) [80, 81] as lattice clock candidates. Because the electronic structure is very similar for all atoms with two valence electrons, the lattice clock scheme could in principle be employed with Be, Mg, Ca, Ba, Zn, Cd, Ra, and the synthetic element nobelium (No).

In these divalent atoms, the electronic structure can be arranged by symmetry into singlet states and triplet states, and transitions between the two manifolds are generally forbidden. The two clock states are the  $^1S_0$  ground state and the  $^3P_0$  excited state, and the radiative transition between them is both spin- and dipole-forbidden. This gives the excited state a very long lifetime, and potentially allows for the observation of an extremely narrow clock transition, which yields a large  $Q$ -factor as discussed above. In fact, in isotopes lacking nuclear spin, the  $^3P_0$  lifetime has been calculated to be a few thousand years [82]! While a long-lived excited state is an essential ingredient in the lattice clock scheme, this is actually far too long to be useful, because the transition is too weak to efficiently excite.

For this reason, most experiments use an isotope that does have nuclear spin. Here, the hyperfine interaction perturbs the excited clock state ( $^3P_0$ ), mixing it with other nearby states and typically resulting in a hyperfine-quenched  $^3P_0$  lifetime of several tens of seconds [83, 84]. These odd-mass-number isotopes are less abundant than the (spin-0) even-mass-number isotopes, but usually the odd isotopes have sufficient abundance to carry out experiments.<sup>2</sup> The amount of

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<sup>2</sup> One notable exception is Ca, in which the only odd isotope (43) has 0.135 % abundance.

hyperfine quenching in these isotopes is favorable for a high-performance clock, being neither too little (in which case a very high intensity would be required to drive the transition with a laser) nor too much (in which case spontaneous decay could limit the observation of a narrow spectrum). But, while the nuclear spin is beneficial for its hyperfine quenching, it brings several other effects that could be deleterious for high-precision spectroscopy. First, the clock states are no longer purely  $J = 0$ , but instead should be labeled by their total angular momentum  $F = J + I$ . This creates  $2I + 1$  substates in both the ground and excited clock states, each substate with its own sensitivity to magnetic fields through the Zeeman effect. Moreover, the clock transition is not one transition but many.<sup>3</sup> With Sr, the only abundant odd isotope has  $I = 9/2$ , for which the complexity associated with these effects is substantial. Second, the spherical symmetry of the  $J = 0$  state is partially lost, which allows for a small interaction between the atom and the polarization of the lattice light field. While these vector and tensor light shifts are expected to be small, they could be problematic, especially for multidimensional lattice configurations. We will examine these nuclear spin effects in greater detail in Sec. 2.3.

These concerns led researchers to revisit the idea of the ( $I = 0$ ) even isotopes. Several theoretical proposals [85, 86, 87, 88] showed that the addition of an external field (either another light field or a magnetic field) could dramatically increase the transition strength without significantly perturbing the clock transition frequency. Of these, magnetically-induced spectroscopy was investigated experimentally [89, 2], and the prospects for high-accuracy lattice clocks with even isotopes remain promising [90, 91, 92]. The benefits of working with these even isotopes include higher natural abundance, a lack of nuclear substructure, the absence of any optical pumping or Zeeman effects (to first-order), and the lack of vector and tensor light shifts from the lattice. The disadvantage, however, is that the large magnetic field and higher clock laser intensity produce two non-negligible frequency shifts that must be well-calibrated.

The trade-off, then, is between the simplicity of a pure two-level system for which we must

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<sup>3</sup> With  $2I + 1$  substates in both the ground and excited clock state, there are  $2I + 1$   $\pi$ -transitions (i.e.  $\Delta m_F = 0$ ), and  $4I$   $\sigma$ -transitions (i.e.  $\Delta m_F = \pm 1$ ).

calibrate two substantial frequency shifts, or the beauty of a naturally-enabled transition that comes with the additional complexity of nuclear substructure. But, suppose the nuclear spin was small,  $I = 1/2$  being the smallest. Then, there are only two ground states and two excited states, between which we could drive two  $\pi$ -transitions or two  $\sigma$ -transitions. This makes first-order Zeeman shifts and optical pumping more straightforward to control. Moreover, one can show that one of the substate-dependent light shifts (namely the tensor shift) is absent for this special case [41]. Thus, a spin-1/2 isotope enjoys many of the benefits of both higher- and zero-angular momentum systems, and, provided the vector light shift can also be controlled well, seems optimally suited for high-accuracy optical spectroscopy.

In addition to the choice of isotope (even or odd), the particular atomic species that performs best as a lattice clock is so far unsettled. Sr and Yb offer the simplest route to a functional lattice clock, with accessible cooling transitions capable of reaching ultracold temperatures and laser requirements that can be met with standard technologies. Hg is more difficult because the relevant laser wavelengths lie in the ultraviolet; however, it has enough tantalizing properties (notably a small sensitivity to blackbody radiation [80]; see Ch. 6) to warrant experimental investigation. While not currently being investigated as a lattice clock per se, Mg [93, 94, 95] and Ca [96, 97, 98, 99, 100] continue to be studied experimentally for other types of (less precise) timekeeping. In this thesis we will consider mainly the Yb atom. An energy level diagram for the lowest-lying states in Yb is given in Fig 1.1 (c). In addition to the aforementioned clock states, a few other relevant excited states are also given in the figure: cooling transitions from the ground state to  $^1P_1$  and  $^3P_1$  at 399 nm and 556 nm, respectively, and a repumping transition  $^3P_0 \rightarrow ^3D_1$ .

Yb has several properties that make it an appealing choice. For one, several of the essential laser systems can be reached with solid-state and fiber laser systems that, while somewhat expensive, are generally more robust and easier to use than diode lasers. These lasers become especially appealing when faced with the task of making a portable apparatus for terrestrial or space-born applications. Another feature is that the laser cooling does not require repumping lasers [101, 102], and narrow-line cooling with odd isotopes does not require a “stirring” laser to randomize the mag-

netic substate [103]. Yet another advantage to Yb is that it has many stable isotopes. Table 1.1 gives the seven stable isotopes of Yb, along with each isotope’s natural abundance, nuclear spin, and magnetic moment. Because the even-numbered isotopes also have an even number of neutrons, these atoms are bosonic. By contrast, the two odd isotopes (171 and 173) are fermions, and they have nuclear spin as mentioned above. Importantly, Yb does indeed have a spin-1/2 isotope,  $^{171}\text{Yb}$ . The same is true for lattice clock candidates Hg and Cd, to which many of the results presented in this thesis may be highly applicable.

Table 1.1: The seven stable isotopes of Yb are given, along with the natural abundance, nuclear spin, and magnetic moment of each [104].

| Isotope           | Abundance | Nuclear spin | Magnetic moment |
|-------------------|-----------|--------------|-----------------|
| $^{168}\text{Yb}$ | 0.13%     | 0            | 0               |
| $^{170}\text{Yb}$ | 3.05%     | 0            | 0               |
| $^{171}\text{Yb}$ | 14.3%     | 1/2          | +0.4919         |
| $^{172}\text{Yb}$ | 21.9%     | 0            | 0               |
| $^{173}\text{Yb}$ | 16.12%    | 5/2          | −0.6776         |
| $^{174}\text{Yb}$ | 31.8%     | 0            | 0               |
| $^{176}\text{Yb}$ | 12.7%     | 0            | 0               |

## 1.5 Thesis overview

In Ch. 2, we will examine a few of the basic physical principles that are instrumental to the design and operation of all lattice clocks. In particular, we will consider how neutral atoms are trapped by an off-resonant laser field, and how this confinement suppresses the Doppler and recoil frequency shifts that limit the accuracy of free-space interrogation techniques. The technique that (largely) removes clock errors associated with the trapping light — the magic wavelength technique — will be presented. Next, we will look in greater detail at the effects of nuclear spin and how it impacts the choice of isotope for a lattice clock experiment. Finally, we will consider the relevant noise sources that could limit the stability of lattice clocks.

In Ch. 3, some of the most relevant details of the NIST Yb lattice clock experiment will be

discussed. Particular attention will be paid to the cooling and trapping of atoms and their transfer to an optical lattice; atomic spin-polarization, where-in we pump the atoms to one substate of  $^1S_0$ ; the detection scheme, by which we measure the number of atoms in the ground and excited clock states after spectroscopy and determine the excited fraction; and the keys to developing a high-stability standard, notably the efforts to stabilize the clock laser to an optical cavity. One key result presented here is the observation of a 1 Hz optical spectrum width, corresponding to a record  $Q$ -factor of  $5 \times 10^{14}$ .

In Ch. 4, we will look at the effects that the confining lattice light have on the atomic clock states. Particularly, the experiments used to identify the magic wavelength will be presented, along with efforts to measure much smaller but still relevant higher-order terms.

In Ch. 5, the collisions between two fermionic Yb atoms will be considered. The measurements that, together with a quantitative theoretical model, were used to identify  $p$ -wave cold collisions (both elastic and inelastic) will be presented in detail. Importantly, we will show how the effects of collisions can be fully canceled, resulting in the smallest collision shift ever observed in any type of atomic clock.

In Ch. 6, the blackbody radiation shift will be discussed, along with a high-accuracy measurement of the Yb atom's d.c. polarizability (that is, its sensitivity to static electric fields). With an uncertainty of 21 parts-per-million, this polarizability measurement ranks among the most precise measures of any polarizability to date, and directly reduces the clock uncertainty due to the blackbody radiation shift.

Finally, in Ch. 7, we will look at the Yb clock's full performance, both through internal evaluations of systematic effects, as well as through comparisons with other optical and microwave clocks at NIST. The thesis concludes with the outlook for lattice clocks and Yb in particular.

## Chapter 2

### Optical Lattice Clocks: Underlying Physical Principles

The aim of this chapter is to describe some of the physics that enables optical lattice clocks. In particular, we want to show how one can observe the extremely narrow atomic spectra upon which the clock is based. Two key ideas will emerge, first that frequency shifts associated with the motion of the atom can be suppressed with tight confinement in a harmonic potential (Sec. 2.1), and second that the perturbations caused by this tight confinement can be minimized by choosing an optical potential at a specific wavelength (Sec. 2.2). With these techniques, narrow atomic spectra can indeed be observed, provided there is some mechanism that enables the atom to undergo a highly-forbidden transition, which in this case is provided by the nuclear spin (Sec. 2.3). The chapter concludes with a discussion of the stability that results from a clock based on a narrow optical spectrum (Sec. 2.4).

#### 2.1 Doppler- and recoil-free spectroscopy

Each time a firetruck passes by, sirens blaring, the Doppler effect can be observed as the change in pitch one hears depending on whether the firetruck is approaching or receding. As the source moves toward (away from) the observer, subsequent wave crests are emitted closer to (farther from) the observer, which increases (decreases) the rate at which the observer hears them. Of course, the Doppler effect is present for all wave phenomena, including light waves interacting with moving atoms. An atom moving at 1 m/s parallel to a near-resonant visible laser field experiences a Doppler shift of order 1 MHz – a very large shift by clock standards! For a gas of atoms with



temperature  $T$ , the velocities are Gaussian distributed according to Maxwell-Boltzmann statistics. Since each velocity carries its own Doppler shift, the absorption spectrum is inhomogeneously broadened beyond the transition's natural linewidth.

A second effect experienced by the atom is that of photon recoil. The photon, when absorbed by the atom, carries  $\hbar k$  ( $\vec{k}$  the wavevector) worth of momentum. The kinetic energy associated with that momentum gives rise to the photon recoil shift, which pulls absorption spectra to the blue. Altogether, the apparent absorption frequency for an atom moving with velocity  $\vec{v}$  (in the lab frame) is

$$\omega_v = \omega_0 + \vec{v} \cdot \vec{k} + \frac{\hbar k^2}{2m} \quad (2.1)$$

and the Gaussian absorption profile for the Doppler-broadened ensemble has a full width at half maximum (FWHM)

$$\Delta\omega(T) = \sqrt{\frac{8k_B T \ln(2)}{m}} \frac{2\pi}{\lambda_0} \quad (2.2)$$

with  $k_B$  Boltzmann's constant,  $\lambda_0 = \frac{2\pi c}{\omega_0}$  and  $m$  the atom mass. At room temperature, the Doppler width is  $\sim 500$  MHz, which is far too broad for precision timekeeping. Below, we review several techniques for suppressing the Doppler and recoil effects.

### 2.1.1 Interrogation of free atoms

Several methods exist for reducing Doppler shifts and Doppler broadening. One is saturated spectroscopy, which uses two anti-parallel laser beams to resonantly address a certain velocity class and cancel the Doppler shift [105, 106]. While this technique remains ubiquitous for referencing a laser to a strong atomic transition, it is less effective as a tool for clock spectroscopy because of the inevitably incomplete cancelation of the Doppler shift<sup>1</sup> and because it cannot address all velocity classes simultaneously.

A better approach is to reduce the atomic temperature, which is most easily done with laser cooling. Indeed, since its first demonstration in 1985 [12, 11], laser cooling of atoms has become the most powerful technique in an atomic physicist's toolbox. The most prevalent type of laser cooling

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<sup>1</sup> not to mention the second-order Doppler effect

is denoted “Doppler cooling” because it harnesses the Doppler shift to influence atomic absorption, creating an environment in which the atom preferentially absorbs from a beam of light opposing its motion over a beam parallel to its motion. The resulting kicks of momentum slow the atom just a little, and repeated absorption and re-emission of photons can continue to remove kinetic energy and slow the atom. The Doppler temperature  $T_D$  sets a limit to the effectiveness of Doppler cooling, and it is written

$$T_D = \frac{\hbar \Gamma}{2 k_B} \quad (2.3)$$

with  $\Gamma$  the spontaneous decay rate of the cooling transition. For strong dipole transitions, the Doppler limit might be a few hundred micro-Kelvin. But with other techniques (such as Sisyphus cooling, resolved sideband cooling, or narrow line cooling) it’s often straightforward to reach temperatures of a few micro-Kelvin or less. For a temperature of  $10 \mu\text{K}$ , the Doppler-broadened width is  $\sim 100 \text{ kHz}$  – much reduced from room temperature, yet still too broad for precision spectroscopy (see Fig. 2.1). However, Doppler-free techniques employed with a cold atom sample can be more effective.

Particularly noteworthy is the technique employed in Ca optical clocks, which uses a sequence of four short pulses (two each from two opposing beams) in a Ramsey scheme to suppress both the Doppler and recoil shifts. However, the Doppler cancelation remains imperfect due to wavefront mismatch between the opposing beams and gravitational acceleration of the atoms. Additionally, photon recoil causes spectral line asymmetries and resolution-dependent frequency shifts. Both mechanisms cause residual uncertainties exceeding  $10^{-15}$ , limiting the achievable accuracy of optical standards based on free atoms [107, 108, 96, 109, 110].

### 2.1.2 Interrogation of confined atoms

Suppose instead that the atom was harmonically confined during spectroscopy. To see how the absorption spectrum is altered by the confinement, we begin by writing the combined Hamiltonian

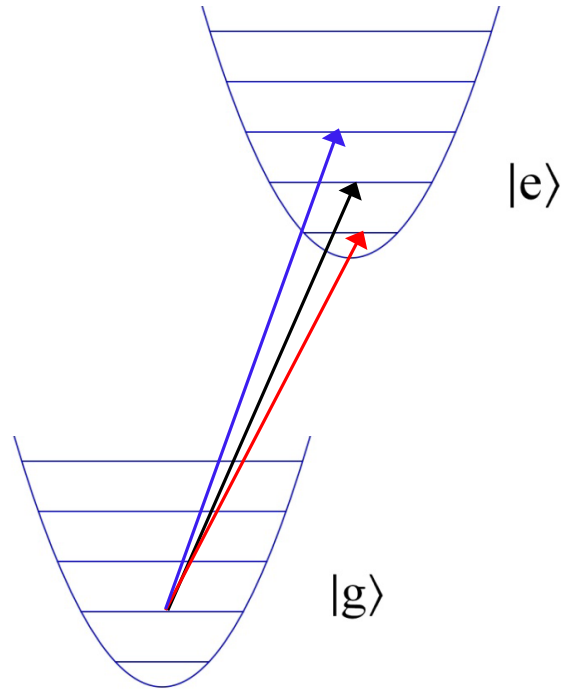
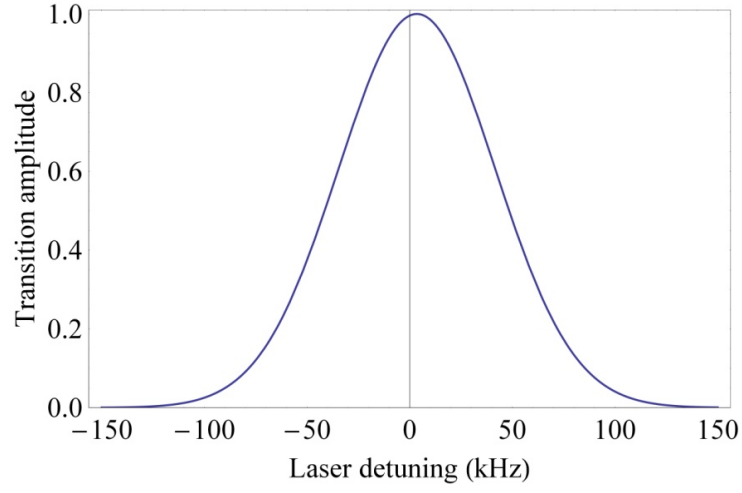


Figure 2.1: Top: The Doppler-broadened and recoil-shifted absorption spectrum of a free atom at  $T = 10 \mu\text{K}$ . Even at this ultracold temperature, the Doppler width  $\Delta\nu$  is nearly 90 kHz. Here,  $\omega_r/2\pi = 3.5$  kHz as in Yb. Bottom: A harmonically-bound atom undergoes quantized motion. Hence, its absorption spectrum is restricted to discrete values. Shown are the “carrier” transition (pure electronic excitation) in black; first red sideband in red; and first blue sideband in blue.

for the electronic structure and harmonic confinement:

$$H^{(0)} = H^{El} + H^{HO} \quad (2.4)$$

$$H^{El} = \hbar(\omega_g |g\rangle\langle g| + \omega_e |e\rangle\langle e|) \quad (2.5)$$

$$H^{HO} = \hbar\omega \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right). \quad (2.6)$$

The atom's electronic states are  $|g\rangle$  and  $|e\rangle$  and have energy  $\hbar\omega_{g,e}$ ;  $\omega$  is the harmonic oscillator frequency. The familiar creation and annihilation operators have been used to express the harmonic potential. The eigenstates of  $H^{(0)}$  are simple products of the internal electronic states ( $|g\rangle$  and  $|e\rangle$ ) and harmonic oscillator ladder states (denoted  $|n\rangle$ ).

We now include an interaction between the confined atom and a resonant light field:

$$H^{(1)} = \frac{\hbar\Omega_0}{2} \left( e^{-ik\hat{x}+i\omega_L t} |g\rangle\langle e| + e^{ik\hat{x}-i\omega_L t} |e\rangle\langle g| \right) \quad (2.7)$$

where  $\Omega_0$  is the Rabi frequency of the light-atom interaction, itself a product of the atomic dipole moment and the laser's electric field. Note that the rotating wave approximation has been made.

The eigenstates of the combined Hamiltonian ( $H^{(0)} + H^{(1)}$ ) are superpositions of the product states mentioned above. The solution to the Schroedinger equation is a generalized Rabi flopping between the states  $|n, g\rangle$  and  $|m, e\rangle$  (see Ref. [111] for the full solutions). For  $n = m$ , the transition is purely electronic and is labeled the carrier transition; for  $n \neq m$ , the transition includes both electronic excitation and a change in motional state, as the atom is driven up or down the harmonic ladder. Of particular interest is the Rabi frequency, which can be written

$$\frac{\Omega_{mn}}{\Omega_0} = \begin{cases} e^{\frac{-\eta^2}{2}} \sqrt{\frac{n!}{m!}} \eta^{m-n} L_n^{m-n}(\eta^2) & \text{if } m > n \\ e^{\frac{-\eta^2}{2}} L_n^0(\eta^2) & \text{if } m = n \\ e^{\frac{-\eta^2}{2}} \sqrt{\frac{m!}{n!}} \eta^{n-m} L_m^{n-m}(\eta^2) & \text{if } n > m \end{cases} \quad (2.8)$$

with  $L_a^n(x)$  the generalized Laguerre polynomial.  $\eta = \sqrt{\omega_r/\omega} = k_0 x_0/\sqrt{2}$  is the Lamb-Dicke parameter, which compares the trap frequency  $\omega$  to the recoil frequency  $\omega_r$ , or, equivalently, the spatial extent of the confined atom ( $x_0 = \sqrt{\hbar/m\omega}$ ) to the transition wavelength  $\lambda_0 = 2\pi/k_0$ . With

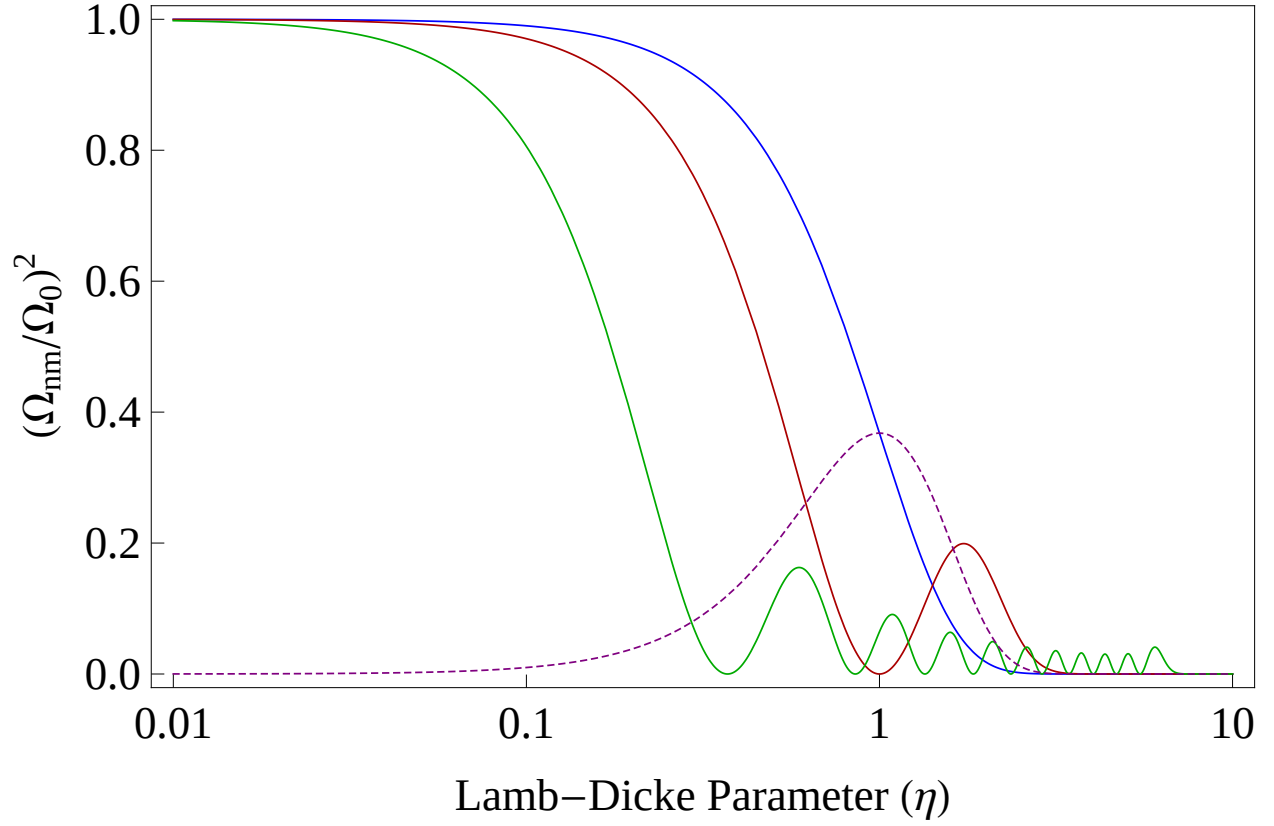


Figure 2.2: Rabi frequency for pure electronic excitation as a function of Lamb-Dicke parameter  $\eta$  for a few different motional states. Blue:  $\Omega_{0,0}$ . Red:  $\Omega_{1,1}$ . Green:  $\Omega_{10,10}$ . Also shown in dashed purple is the sideband  $\Omega_{0,1}$ .

tight confinement, it's possible to achieve  $\eta < 1$ , known as the Lamb-Dicke regime, wherein the atom's spatial extent is smaller than the transition wavelength.

Eq. 2.8 shows that the confined atom will always be excited with a lower Rabi frequency than a stationary atom. This effect is a result of the excitation spectrum being modulated by the atom's harmonic motion, and can be made small by ensuring a deep trap (i.e.  $\eta \ll 1$ ). In the Lamb-Dicke regime, Eq. 2.8 simplifies to

$$\begin{aligned}\Omega_{n,n-1} &= \eta \sqrt{n} \Omega_0 \\ \Omega_{nn} &\rightarrow \Omega_0 \\ \Omega_{n,n+1} &= \eta \sqrt{n+1} \Omega_0\end{aligned}\tag{2.9}$$

Fig. 2.2 shows the Rabi frequency of the carrier transition as a function of  $\eta$  for a few motional states.

To see how harmonic confinement suppresses Doppler and recoil shifts, consider the spectra in Fig. 2.3. There, we see a simulated absorption spectrum for several different trap depths. With very weak confinement, the spectrum looks exactly like a discrete version of the Doppler-broadened and recoil-shifted spectrum in Fig. 2.1. For the weakest case shown, the individual spectra are not resolved, indicating the transition linewidth exceeds  $\omega$ .<sup>2</sup> As the confinement is increased, the sidebands move to higher frequency and become easily resolved, and fewer transitions are observed. Most importantly, we see the presence of an unshifted carrier transition, for which the only recoil effect is line-pulling towards the blue side. At the highest confinement, the carrier dominates the spectrum, and clearly any line-pulling toward the blue sideband is negligibly small.

To generate the spectra, the Rabi frequency for a given transition (i.e. carrier, first sideband, second sideband, etc) was calculated by thermally-averaging Eq. 2.8 over a Boltzmann-distribution

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<sup>2</sup> To be clear, though, in the case of Fig. 2.3, the spectra are treated as delta functions which gain a finite width only when plotted.

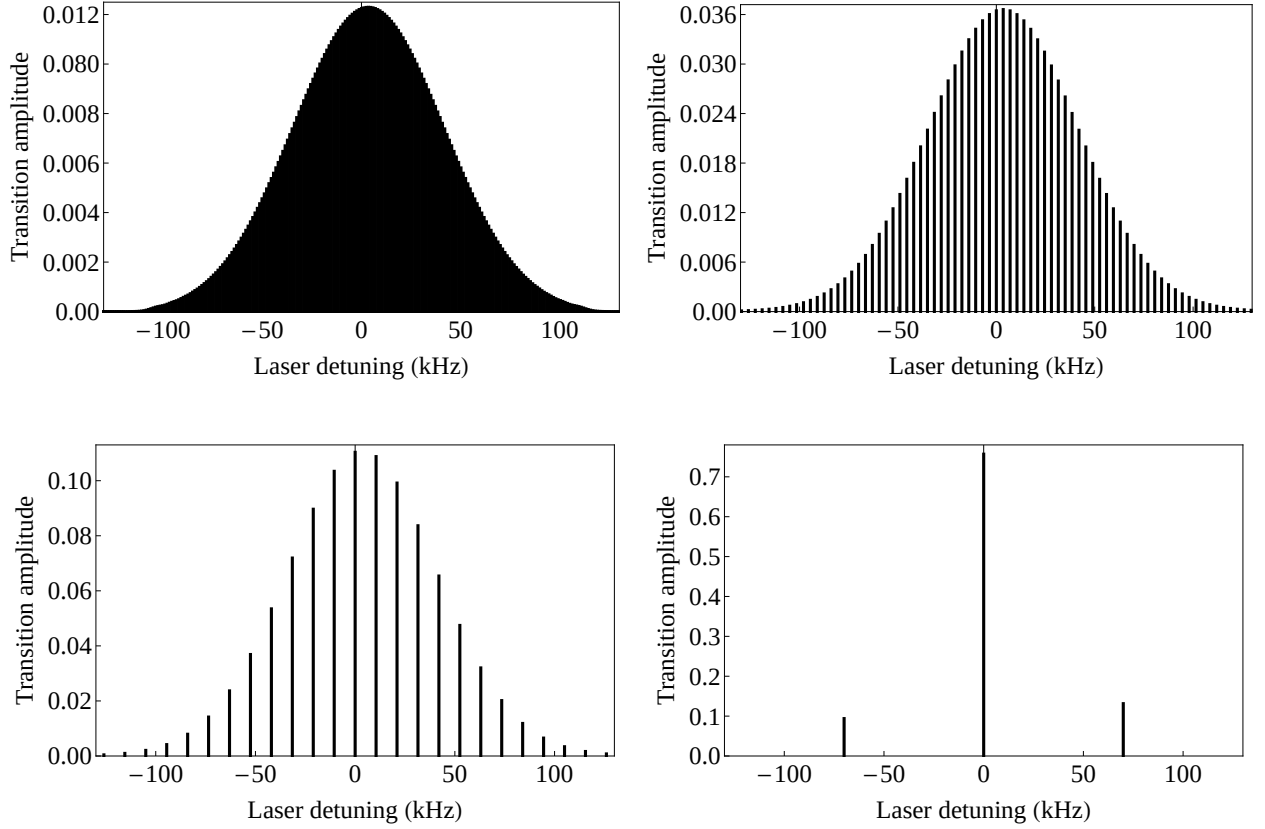


Figure 2.3: Shown are the absorption spectra (specifically,  $\langle(\Omega_{nm}/\Omega_0)^2\rangle_T$ ) for several different confinement strengths. Upper left:  $\omega = \omega_r/3$ . Upper right:  $\omega = \omega_r$ . Lower left:  $\omega = 3\omega_r$ . Lower right:  $\omega = 20\omega_r$ . The plots demonstrate how a deeper trap suppresses sideband amplitudes and line-pulling due to the recoil shift. The spectra were generated for  $T=10\text{ }\mu\text{K}$  and  $\omega_r/2\pi = 3.5\text{ kHz}$ .

of populated motional states. The amplitudes for the  $k^{\text{th}}$  blue and red sidebands are

$$\begin{aligned}
 \text{Blue:} \quad \left\langle \left( \frac{\Omega_{n,n+k}}{\Omega_0} \right)^2 \right\rangle_T &= \frac{\sum_{n=0}^N e^{-\frac{(n+1/2)\hbar\omega}{k_B T}} \left( \frac{\Omega_{n,n+k}}{\Omega_0} \right)^2}{\sum_{n=0}^N e^{-\frac{(n+1/2)\hbar\omega}{k_B T}}} \\
 \text{Red:} \quad \left\langle \left( \frac{\Omega_{n,n-k}}{\Omega_0} \right)^2 \right\rangle_T &= \frac{\sum_{n=k}^N e^{-\frac{(n+1/2)\hbar\omega}{k_B T}} \left( \frac{\Omega_{n,n-k}}{\Omega_0} \right)^2}{\sum_{n=0}^{N_f} e^{-\frac{(n+1/2)\hbar\omega}{k_B T}}}
 \end{aligned} \tag{2.10}$$

with  $N$  the total number of bound states.<sup>3</sup> Notice that the only difference between the two cases is that, for the red sideband, the summation begins at  $n = k$  instead of  $n = 0$  because there are no lower-lying motional states into which the atom can make a transition. This asymmetry in the spectra is a manifestation of the recoil effect.

Having seen that tight harmonic confinement results in a near complete suppression of photon recoil, one might reasonably wonder what happened to the recoil energy, for surely the photon still carries momentum. The answer is that the recoil was absorbed by the potential. In fact, it has been proposed that one could detect when a confined atom makes a transition by precisely measuring the backaction of photon recoil on the optical lattice that forms the potential [112].

## 2.2 Atomic confinement in an optical potential

Near-resonant laser light is extremely useful for atom cooling; however, it cannot be used for trapping atoms during clock spectroscopy because it strongly perturbs the atom's internal states. By contrast, off-resonant light only weakly perturbs the atomic states via the ac Stark shift, and for sufficiently large detuning, the photon absorption (and subsequent re-emission) rate can be quite small. Here we show how off-resonant light is used to make an atom trap.

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<sup>3</sup> Here, the summation was truncated at the  $N$  value when the Boltzmann term became negligibly small. In any real experiment, the trap depth is finite, limiting the number of bound states.



### 2.2.1 The dipole force

Consider an atom in the presence of a laser, oscillating with frequency  $\omega_L$  and electric field amplitude  $\mathcal{E}$ . The electric field induces a dipole moment in the atom, the strength of which depends on the atom's polarizability  $\alpha$ , which is itself a function of  $\omega_L$  and is generally complex. The interaction between the induced dipole moment and the electric field causes an energy shift to the atomic levels. After time-averaging over the oscillation, we find the interaction energy is [113, 41]

$$\begin{aligned} U_0 &= -\frac{1}{4} \text{Re}[\alpha] \mathcal{E}^2 \\ &= \frac{1}{2\epsilon_0 c} \text{Re}[\alpha] I \end{aligned} \quad (2.11)$$

with  $\epsilon_0$  the permittivity of free space,  $c$  the speed of light, and  $I = \frac{1}{2} c \epsilon_0 \mathcal{E}^2$  the laser intensity. The energy shift scales with  $\mathcal{E}^2$  because the field is responsible for inducing, and interacting with, the dipole moment.

Eq. 2.11 gives the potential energy of the atom-laser interaction. To have a non-zero force acting on the atom, there must be a spatial gradient in the potential: [113]

$$\vec{F} = \frac{1}{2\epsilon_0 c} \text{Re}[\alpha] \vec{\nabla} I. \quad (2.12)$$

While the dipole force depends on the real part of the atom's polarizability (because it is a dispersive interaction), the imaginary part gives the photon absorption and re-scattering rate, which can heat the atom and limit the dipole trap lifetime. The photon scattering rate is written

$$\gamma_s = \frac{\text{Im}[\alpha]}{\hbar \epsilon_0 c} I \quad (2.13)$$

The polarizability of a two-level atom can be found in a semi-classical way by treating the electron as a driven harmonic oscillator, where the harmonic frequency matches that of the atomic transition  $\omega_0$ , and damping is given by the spontaneous decay rate  $\Gamma$  [113]. Solving the harmonic oscillator differential equation for the electron's displacement, we can write the polarizability as

$$\alpha = 6\pi\epsilon_0 c^3 \frac{\Gamma/\omega_0^2}{\omega_0^2 - \omega_L^2 - i(\omega_L^3/\omega_0^2)\Gamma}. \quad (2.14)$$

Multi-level atoms require only a simple summation over the various resonances ( $\omega_m$ ) that connect to the atomic state of interest, denoted  $|i\rangle$ . In the limit of large detuning ( $|\omega_0 - \omega_L| \gg \Gamma$ ), the polarizability is

$$\text{Re}[\alpha_i] = 6\pi c^3 \epsilon_0 \sum_m \frac{\Gamma_m}{\omega_m^2 (\omega_m^2 - \omega_L^2)} \quad (2.15)$$

$$= 3\pi c^3 \epsilon_0 \sum_m \frac{\Gamma_m}{\omega_m^3} \left( \frac{1}{\omega_m - \omega_L} + \frac{1}{\omega_m + \omega_L} \right)$$

$$\text{Im}[\alpha_i] = 6\pi c^3 \epsilon_0 \sum_m \frac{\Gamma_m^2 \omega_L^3}{\omega_m^4 (\omega_m^2 - \omega_L^2)^2} \quad (2.16)$$

where  $\Gamma_m$  is understood to be the decay rate between  $|m\rangle$  and  $|i\rangle$ , and  $\hbar\omega_m$  is the energy splitting between those states. Note that the above equations include the so-called Bloch-Siegert shift, which is needed to correctly describe the interaction of an atom with a far-detuned laser. A sample calculation using these equations is given in Sec. 2.2.3. Typically, when one refers to  $\alpha$  or to the “polarizability”, they mean the real part only, which is the convention we will adopt going forward.

### 2.2.2 An optical lattice

As mentioned above, a spatial gradient in the laser’s intensity distribution is needed to produce a dipole force. With a typical choice of a red-detuned laser, the atoms are attracted to areas of highest laser intensity. For some geometries, this dipole force can be harnessed to produce an atom trap. Here we consider the optical lattice geometry, which is formed from one or more standing wave laser fields. The simplest case is a 1D lattice, wherein intensity maxima are periodically spaced by  $\lambda/2$ , with  $\lambda = 2\pi c/\omega_L$  the laser wavelength, and the atoms are tightly held at the antinodes of the standing wave. Orthogonal to the lattice direction, the Gaussian shape of the laser beam provides confinement, albeit weaker than along the lattice direction. For this reason, the laser intensity (and the atoms’ wavefunctions) in a 1D lattice resembles a stack of pancakes.

Typically, the standing wave is formed by retroreflecting a focused laser beam (with suitable optics to match the beam parameters of the forward-going beam). Near the focus, we can write

the time-averaged trapping potential as

$$\langle U(r, z) \rangle = -U_0 \cos^2(2\pi z/\lambda) e^{-2r^2/w_0^2} \quad (2.17)$$

with  $r$  the radial coordinate,  $z$  the direction of laser propagation,  $w_0$  the Gaussian beam's  $1/e$  field radius, and  $U_0$  defined in Eq. 2.11. We can also relate the trap depth to the (one-way) optical power ( $P$ ) as

$$U_0 = \frac{4\alpha_i P}{c\epsilon_0\pi w_0^2} \quad (2.18)$$

with  $\alpha_i$  the polarizability of state  $|i\rangle$ . Note that the factor of 4 is due to constructive interference between the two counter-propagating beams, assuming their polarization vectors are matched.

Now, we can make an approximation, one that is familiar to physicists: we pretend that lattice potential is harmonic. Setting the potential in each direction equal to the well-known harmonic oscillator potential ( $V(x) = \frac{1}{2}m\omega_x^2 x^2$ , with  $m$  the atom mass), we find the radial and longitudinal vibrational frequencies,  $f_R$  and  $f_L$ , respectively [114, 115]:

$$f_R = \frac{1}{\pi w_0} \sqrt{\frac{U_0}{m}} \quad (2.19)$$

$$f_L = \frac{1}{\lambda} \sqrt{\frac{2U_0}{m}}. \quad (2.20)$$

Notice the ratio of the two trap frequencies is independent of the trap depth and depends only on the spot size. Of course, the potential is not truly harmonic, but it turns out to be a good approximation for the lowest vibrational states. We will consider anharmonicity in the next subsection.

A 1D lattice is primarily used throughout this thesis, but for a handful of measurements, a 2D lattice was employed. The 2D lattice comes in many varieties based on several key design choices. For one, should the 2D lattice be formed from one light source or two? In the former case, a single beam is steered to intersect the atomic cloud from two (or three) directions, and folded on itself to form a standing wave. This method has several benefits, ranging from an efficient use of laser power to the “topological stability” described in several references <sup>4</sup> [116, 117, 118, 119].

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<sup>4</sup> Briefly, in multi-dimensional lattices, we must consider the relative phases of the intersecting beams. A folded-beam 2D lattice is guaranteed to preserve the shape of the interference pattern even when mirror vibrations change the optical path length. By contrast, the same mirror vibrations can distort the interference pattern formed by independent beams.

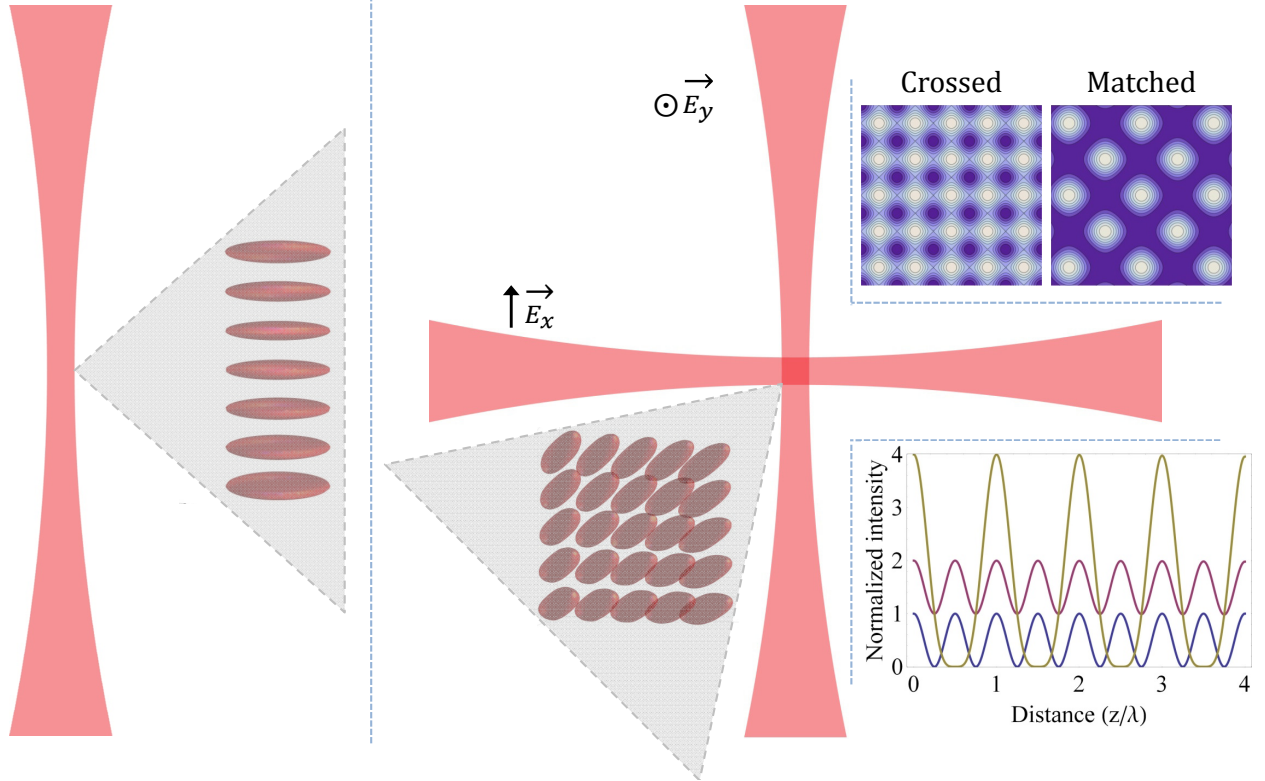


Figure 2.4: Left: A 1D lattice resembles a stack of “pancakes”. Right: A 2D lattice with crossed polarization. Here the lattice sites resemble tubes (“French toast sticks”). Upper right: Contour plots of crossed and matched 2D lattices. Lower left: Plotted is a line-out of the intensity distribution (through the center of the lattice sites) for a 1D lattice (blue), a crossed 2D lattice (purple) and a matched 2D lattice (gold).

Alternatively, the 2D lattice can be formed from separate laser sources. While this method requires more optical power, and is more sensitive to phase fluctuations (caused by relative vibrations of the retroreflectors), it brings additional flexibility compared to the folded beam lattice. Specifically, the amplitude, polarization, and frequency of each dimension of lattice can be controlled independently. In the Yb experiment, we have used this flexibility in several ways, including protocols to ensure true two-dimensional confinement (see Sec. 3.2) and to help control spurious effects from the vector Stark shift (see Sec. 2.3 and 4.4).

Another key design choice of the 2D lattice is whether the two dimensions should have the same polarization or not. If the polarizations are crossed, there is no interference between the two beams, and a rectangular grid of lattice sites results. Of course, if the polarizations are matched, the beams will interfere; this creates a deeper trap due to the additional constructive interference (if the frequencies are also matched). In addition (and somewhat counterintuitively), it also modifies the spatial distribution of lattice sites. We can see this by examining the potential (here assuming equal amplitude and frequency for the two lattice dimensions, as well as linear polarization)[117]:

$$\begin{aligned} \langle U(x, y, z) \rangle = & -U_0 e^{-2z^2/w_0^2} \left( \cos^2 \left[ \frac{2\pi x}{\lambda} \right] e^{-2y^2/w_0^2} + \cos^2 \left[ \frac{2\pi y}{\lambda} \right] e^{-2x^2/w_0^2} \right. \\ & \left. + 2 \vec{e}_1 \cdot \vec{e}_2 \cos(\phi_T) \cos \left[ \frac{2\pi x}{\lambda} \right] \cos \left[ \frac{2\pi y}{\lambda} \right] e^{(-x^2-y^2)/w_0^2} \right). \end{aligned} \quad (2.21)$$

Here,  $\vec{e}_1$  and  $\vec{e}_2$  give the polarizations of the two beams, and their dot product determines whether the 2D lattice is formed by two independent standing waves or by a mutually-interfering composite wave. In the latter case, we also must consider the relative time-phase (denoted by  $\phi_T$ ) between the two standing waves [116, 117]. Obviously, if at one instant in time, one standing wave has maximal intensity while the other does not, the interference between the two waves is reduced.

In the case of the crossed-polarization geometry, the total intensity at each lattice site is twice as high as for a 1D lattice; however, the trap depth is not increased due to the transverse extent of the other beam (see the intensity cross-section depicted in Fig. 2.4).

In the matched polarization case, the additional interference produces components of spatial frequency  $k = 2\pi/\lambda$  in addition to those at  $2k$ . We can see this by writing the potential in a slightly

different form [116]:

$$\begin{aligned}\langle U(x, y, z) \rangle &= -U_0 (\cos[kx] + \cos[ky])^2 \\ &= -4U_0 \cos^2\left[\frac{k}{2}(x+y)\right] \cos^2\left[\frac{k}{2}(x-y)\right].\end{aligned}\tag{2.22}$$

Here the Gaussian extent of each beam has been omitted for simplicity (i.e. the above equation applies only at the central lattice sites) and we have taken  $\cos\phi_T = 1$ . The spacing between adjacent lattice sites is  $\lambda$  (along one of the lattice directions), and the shape of the intensity distribution resembles a  $\cos^4$  function. Because of the added complication of potential depth depending on the time-phase term ( $\phi_T$ ), we chose to use a crossed lattice geometry for the 2D lattice experiments described throughout the thesis.

For any of the trapping geometries discussed above, we require that the trap depth, easily expressed as a temperature by dividing out Boltzmann's constant  $k_B$ , exceed the atomic temperature in order for a reasonable fraction of atoms to be trapped. For Yb, a 1D lattice with intensity of  $140 \text{ kW/cm}^2$  produces a trap depth of about  $50 \text{ } \mu\text{K}$ , while it is straightforward to achieve atomic temperatures of  $15 \text{ } \mu\text{K}$  with laser cooling (see Ch. 3). Another common unit for expressing the lattice depth is in terms of the lattice photon recoil energy. For Yb,  $E_r \simeq 2 \text{ kHz}$ , so a lattice depth of  $50 \text{ } \mu\text{K}$  equates to  $\simeq 500 E_r$ .

### 2.2.3 Stark shift cancelation and uniform confinement

We have seen how an optical lattice provides tight atomic confinement via the ac Stark shift. While this is very beneficial for suppressing the Doppler and recoil shifts, the drawback is that the atom's internal levels are perturbed in a non-trivial way. The clock frequency, as observed by the energy splitting between the ground and excited state, is now a function of the lattice laser's intensity, polarization, and wavelength.

Figure 2.5: Low-lying states of Yb, arranged by term symbol. The base configuration is  $[\text{Xe}]4f^{14}$ . The states are arranged by symmetry into two manifolds (singlet, shown here at the left, and triplet, shown at the right). States with odd parity are marked with  $^{\circ}$ . Also shown is one of the many inner-shell excitations:  $4f^{13}(^2F_{7/2})5d_{5/2}6s^2(j=1)$ . This state is noteworthy because it has a non-zero matrix element with the ground state. Note also the doubly-excited  $6p^2\ ^3P_J$  states (marked with an asterisk), which have even parity; thus, the matrix element between  $6p^2\ ^3P_1$  and the excited clock state is also non-zero. The dashed gray line at the top shows the ionization potential ( $\sim 6.3$  eV), although it should be noted that there are an abundance of states (not shown) that lie just beneath this line [104].

Table 2.1: List of states used to calculate the dynamic polarizability and magic wavelength in Yb. Taken from [92], which gathered energy splittings from [104] and lifetimes from [120, 121, 122]. Branching ratios for low-lying states were calculated under  $L - S$  coupling, while those for higher-lying states were estimated according to  $\omega^3$  scaling.

States used in calculating  $^1S_0$  polarizability

| State            | Energy ( $\text{cm}^{-1}$ ) | Lifetime (ns) | Branching Ratio | Fractional contribution |
|------------------|-----------------------------|---------------|-----------------|-------------------------|
| 6s6p $^1P_1$     | 25068.222                   | 5.464         | 1               | 77.3 %                  |
| 6s7p $^1P_1$     | 40563.97                    | 9.2           | 0.80            | 4.3 %                   |
| 6s8p $^1P_1$     | 44017.60                    | 43            | 0.65            | 0.5 %                   |
| 6s6p $^3P_1$     | 17992.007                   | 870           | 1               | 3.0 %                   |
| (7/2, 5/2) $j=1$ | 28857.014                   | 14.6          | 1               | 15.0 %                  |

States used in calculating  $^3P_0$  polarizability

| State           | Energy splitting ( $\text{cm}^{-1}$ ) | Lifetime (ns) | Branching Ratio | Fractional contribution |
|-----------------|---------------------------------------|---------------|-----------------|-------------------------|
| 6s7s $^3S_1$    | 15406.253                             | 14            | 0.15            | 92.5 %                  |
| 6s8s $^3S_1$    | 24326.601                             | 34            | 0.135           | 1.9 %                   |
| 6s5d $^3D_1$    | 7200.663                              | 376           | 0.639           | -25.1 %                 |
| 6s6d $^3D_1$    | 22520.281                             | 21            | 0.582           | 19.2 %                  |
| 6s7d $^3D_1$    | 27022.941                             | 38            | 0.56            | 4.2 %                   |
| 6p $^2$ $^3P_1$ | 26516.981                             | 15            | 0.35            | 7.3 %                   |



Of course, one could always hope to measure and correct for this lattice shift. But to be well into the Lamb-Dicke regime ( $2\pi f_L \gg \omega_r$ ) requires trap depths of order 100 kHz; even with part-per-thousand knowledge of the lattice light shift, the clock’s uncertainty exceeds  $10^{-13}$ . Moreover, the atoms in higher motional bands of the lattice spend less time near the trap center than the atoms in lower bands, meaning they see a lower lattice intensity on average. Thus the Stark shift is different for each motional state, and the confining lattice potential is a source of inhomogeneous spectral broadening, degrading both the clock’s stability and accuracy.

But there is a better way. Suppose we could find conditions under which the ground and excited states were uniformly confined. Then, to first-order in intensity, the Stark shift on the two levels is identical, and the *net* Stark shift vanishes. This is precisely the case for the  $^1S_0$  and  $^3P_0$  states in alkaline-earth atoms, which have a level diagram similar to that shown in Fig. 2.5. For a lattice wavelength to the red of the  $^3S_1 \leftrightarrow ^3P_0$  transition but to the blue of the  $^3D_1 \leftrightarrow ^3P_0$  transition, there exists a “magic” wavelength where the clock states have the same polarizability, and the net Stark shift vanishes. One key piece in this scheme is the scalar nature of the  $J = 0$  clock states, which minimizes the dependence on the polarization of the lattice laser [40].<sup>5</sup> This is important because optical polarization can be one of the more difficult parameters to control experimentally.

To calculate the magic wavelength, we use Eq. 2.15 to first calculate the polarizability for both clock states as a function of  $\lambda$ . For each resonance summed over, the decay rate  $\Gamma_m$  is given by the inverse of the upper state’s lifetime, divided by the fraction that decays into the clock state (i.e. the branching ratio, which is calculated from angular momentum considerations [123].) Fig. 2.6 shows the calculated polarizability for the ground and excited clock states in Yb, using the higher-lying states (and their respective energy splittings, lifetimes, and branching ratios) listed in Table 2.1. These numbers were taken from [92].

The magic wavelength is given by the intersection of the two curves, which is shown in the lower panel of Fig. 2.6 near 742 nm. While the energy splittings are known with high accuracy, the lifetimes and branching ratios are not. Moreover, the two curves cross at a flat angle, which

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<sup>5</sup> In fact, for bosonic isotopes, the light shift is independent of the optical polarization, to first order in  $I$ .

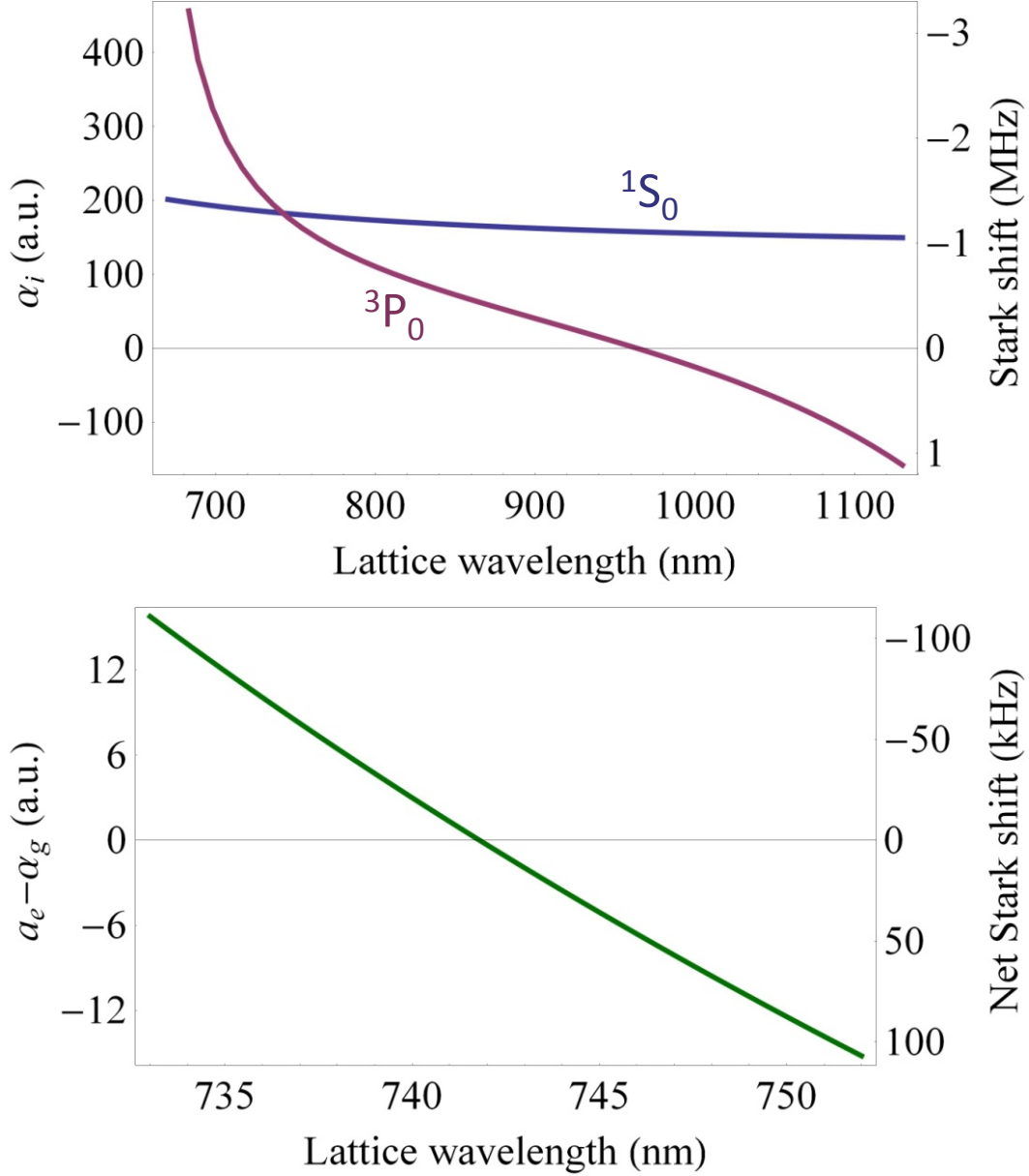


Figure 2.6: Top: Calculated polarizability in atomic units [124] for the ground and excited clock states in Yb. The curves cross near  $\lambda_{\text{magic}} \approx 742$  nm. The right axis gives the Stark shift for an intensity  $I = 140$  kW/cm<sup>2</sup>. Bottom: Subtracting the 2 curves above, we find the *differential* polarizability and the *net* Stark shift.

makes the calculation even less accurate. Experimentally, we have observed the magic wavelength at 759.4 nm, which suggests the calculation is accurate to within 2 %. We have also observed that excursions from the magic wavelength cause clock errors with a coefficient of 1 Hz clock shift for 100 MHz lattice shift (for a maximum trap depth of 1 MHz or 50  $\mu$ K), which agrees well with the calculation. Fortunately, this coefficient is small enough that it is straightforward to satisfy the requirements on the frequency stability of the lattice laser. With the same atomic data and with Eq. 2.13 and 2.16, the photon scattering for  $I = 140 \text{ kW/cm}^2$  is  $\gamma_s \sim 0.1/\text{s}$ , which is small enough to be of little concern.

Finding the magic wavelength is not quite the whole story when considering lattice light shifts. Higher-order Stark shifts, arising from two-photon resonances [40, 125, 126] or magnetic dipole transitions [127], are discussed in Ch. 4. For isotopes with nuclear structure, the hyperfine interaction moves the magic wavelength a small amount. More significantly, it also reintroduces some dependence on the optical polarization (since the clock states are no longer pure  $J = 0$ ), giving rise to vector and tensor light shifts, as discussed in Sec. 2.3 and 4.4.

#### 2.2.4 A few complications

A magic wavelength optical lattice is, in many ways, an ideal environment for precision spectroscopy, providing both a strong suppression of frequency shifts from atomic motion and a strong suppression of the perturbation caused by the lattice itself. In a sense, the atom's internal and external degrees of freedom have been separated since the lattice (mostly) does not perturb the atom's energy level spacing. In this section, we consider some ways in which this separation breaks down, allowing the finer details of the lattice confinement to affect the operation of the clock. In particular, we will see how atomic motion within a lattice site affects the carrier and sideband transitions, and we will consider the role of atomic motion between lattice sites via tunneling.

#### 2.2.4.1 How atomic motion affects the carrier: excitation inhomogeneity

According to Eq. 2.2, the confined atom is excited with a Rabi frequency that depends on the atom's motional state  $|n\rangle$ . For a single atom or ion, this does not cause much difficulty, because the bare Rabi frequency  $\Omega_0$  can be tuned by controlling the power of the clock laser to yield spectra with maximal contrast (i.e. a  $\pi$ -pulse for typical Rabi spectroscopy). However, with an ensemble of atoms distributed over many motional states, each atom has a different Rabi frequency, which prohibits a uniform excitation process. This dephasing has been termed “excitation inhomogeneity” [128, 129]. As the spectroscopic process unfolds, atoms initially prepared in the same state will gradually reach different superpositions of the two clock states. For sufficiently high inhomogeneity (or sufficiently long interrogation), the end result is an incoherent 50/50 mixture.

From the perspective of an individual atom, the light-matter interaction is fully coherent, and for that reason the excitation inhomogeneity does not lead to broadening of spectral lines, but rather to reduction of amplitude contrast. But, for two atoms in the same lattice site but different motional states, the differing internal state (given by different superpositions of  $|g\rangle$  and  $|e\rangle$  for each atom) indicates the two atoms are distinguishable. This has important implications for the collisional processes between the two atoms, as discussed in Ch. 5.

For a probe beam that is perfectly aligned along the lattice axis ( $\hat{z}$ ), the Lamb-Dicke parameters along the transverse directions ( $\eta_x = \vec{k}_p \cdot \hat{x} x_0 / \sqrt{2}$ , and similarly for  $\eta_y$ ) are zero. (Here,  $\vec{k}_p$  is the  $k$  vector of the probe beam). In this case, only the distribution of motional states along the  $z$ -direction is a source of inhomogeneity. However, even with careful alignment to ensure the probe direction overlaps the lattice direction, there will still be a small mismatch due to wavefront curvature and aberrations. Experimentally, we have observed a mismatch angle of 9 mrad. With a radial trap frequency  $f_{x,y} = 530$  Hz and longitudinal trap frequency  $f_z = 78$  kHz, the Lamb-Dicke parameters are  $\eta_x = \eta_y = .023$  and  $\eta_z = 0.21$ .

To quantify the level of inhomogeneity, we can write the effective Rabi frequency for carrier

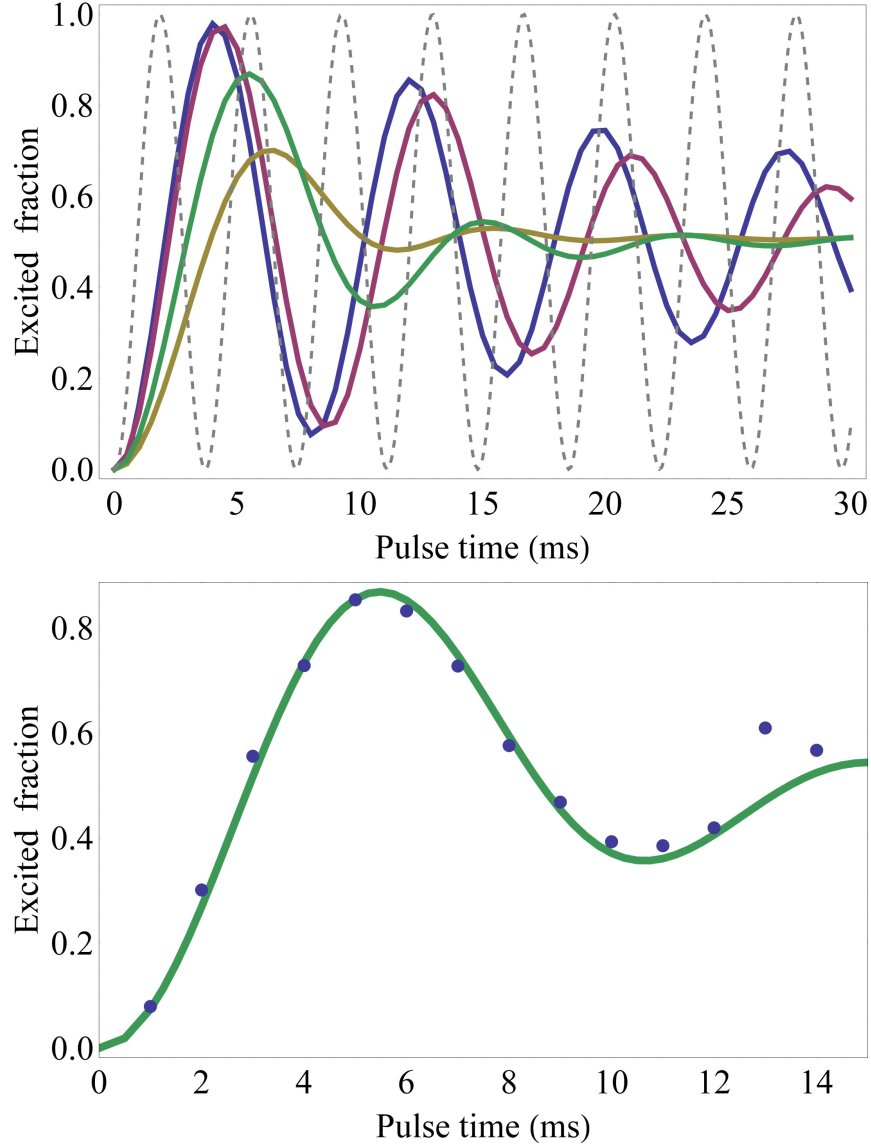


Figure 2.7: As atoms in different motional states are excited on the carrier transition, the spread in Rabi frequencies causes dephasing, which damps the Rabi flopping. Top: Rabi flopping curves for several values of the effective misalignment,  $\Delta\theta$ , with  $T = 9\ \mu\text{K}$ ,  $\Omega_0/2\pi = 135\ \text{Hz}$ ,  $\omega_r/2\pi = 530\ \text{Hz}$ , and  $f_z = 78\ \text{kHz}$ . The blue, purple, green, and gold curves correspond to  $\Delta\theta = \{0, 4, 9, 12\}$  mrad. The dashed grey shows Rabi flopping in the absence of dephasing. Note that even with 0 mrad misalignment, the multiple populated motional states along the lattice direction cause inhomogeneity. Bottom: Points show experimental measurement of the Rabi flopping curve. Solid line is a fit, using  $T = 9\ \mu\text{K}$ ,  $f_{x,y} = 530\ \text{Hz}$ , and  $f_z = 78\ \text{kHz}$ . The result of the summation gives the bare Rabi frequency as  $\Omega_0/2\pi = 135\ \text{Hz}$ , the average Rabi frequency as  $\bar{\Omega}/2\pi = 85\ \text{Hz}$ , the RMS spread as  $\Delta\Omega/2\pi = 22\ \text{Hz}$ , and the thermally-averaged fractional inhomogeneity as  $\left\langle \frac{\bar{\Omega}}{\Delta\Omega} \right\rangle_T = 0.25$ .

excitation in all three-dimensions:

$$\left\langle \frac{\Omega_{\text{eff}}}{\Omega_0} \right\rangle_T = \prod_{i=x,y,z} \frac{\sum_{n_i=0}^{N_i} e^{-\frac{(n_i+1/2)\hbar\omega_i}{k_B T}} e^{-\frac{\eta_i^2}{2}} L_{n_i}^0(\eta_i^2)}{\sum_{n_i=0}^{N_i} e^{-\frac{(n_i+1/2)\hbar\omega_i}{k_B T}}} \quad (2.23)$$

Fig. 2.7 shows a Rabi flopping curve for several different values of the misalignment parameter  $\Delta\theta$ . Even with no misalignment, the Rabi flopping is damped due to the motional state distribution along  $\hat{z}$ . With  $\Delta\theta = 4$  mrad, the additional inhomogeneity from the transverse directions is apparent. The lower panel shows an experimental Rabi flopping curve; overlaid is a theory curve with  $\Delta\theta = 9$  mrad.

The main effects of excitation inhomogeneity are two-fold. First, the signal contrast is reduced from 100%, which potentially limits the  $S/N$  ratio of the spectroscopy. The experimental points in Fig. 2.7 show a maximal contrast just over 80 %. With reduced temperature, tighter confinement, or larger beams, it should be possible to increase this number well above 90 %, after which further progress offers minimal reward. Secondly, and probably of greater significance, is that the atomic population loses its indistinguishability, which can affect both elastic and inelastic collisions, as discussed in Ch. 5.

#### 2.2.4.2 How atomic motion affects the sidebands: anharmonicity and radial coupling

In Fig. 2.3, we considered the sideband structure associated with exciting a bound atom, but we did not include any treatment of the shape of the sidebands. An experimentally measured sideband spectrum is shown in Fig. 2.8. For typical lattice depths, the sidebands are at sufficiently high frequency that only one is visible on each side of the carrier; however, these features look nothing like the narrow, well-defined peaks of Fig. 2.3.

There are two effects that cause the smearing evident in the spectrum. First, the  $\cos^2$  potential is not perfectly harmonic; second, the full 3-dimensional potential (e.g. Eq. 2.17) is not separable into a sum of potentials for the longitudinal ( $z$ ) and radial ( $r$ ) coordinates. Expanding the

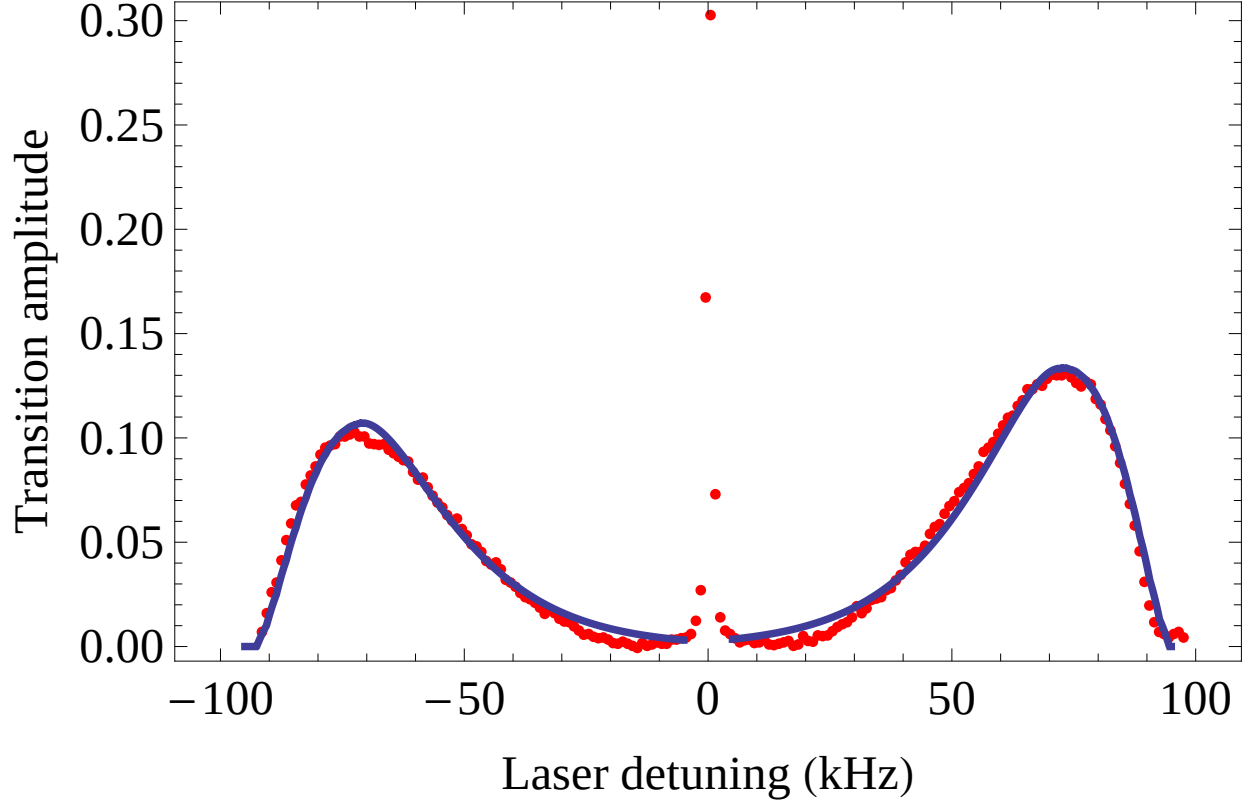


Figure 2.8: The shape of motional sideband spectra shows the effects of anharmonicity and radial coupling. The red points are measurements from the Yb lattice experiment; blue line is the prediction of the model, determined by a best fit with  $A \rightarrow 1275$ ,  $T_R \rightarrow 27.9 \mu\text{K}$ ,  $T_L \rightarrow 17.6 \mu\text{K}$ , and  $\omega/2\pi \rightarrow 96.6 \text{ kHz}$ . At lower trap depths, direct measurements of  $T_R$  suggest  $T_R \sim T_L \approx 10 \mu\text{K}$ .

potential to include harmonic and quartic terms in  $z$ , a harmonic term in  $r$ , and the first coupling term between  $z$  and  $r$ , one finds [129]

$$\langle U(r, z) \rangle \simeq -U_0 \left( 1 - k^2 z^2 + \frac{1}{3} k^4 z^4 - \frac{2 r^2}{w_0^2} + \frac{2 k^2 z^2 r^2}{w_0^2} \right) \quad (2.24)$$

which can be treated with first-order perturbation theory to yield an approximate expression for the energy spectrum (see [129]). Fig. 2.9 shows a dispersion diagram for a trap depth of  $300 E_r$  ( $E_r$  the recoil energy associated with a lattice photon), typical for the Yb experiment. The figure shows energy levels both for a pure harmonic potential and the harmonic + quartic term (but in both cases ignoring the radial coupling). Also plotted in the figure is the solution offered by the Mathieu equation [130], which also ignores radial coupling but is useful for calculating tunneling rates.

The main effect of the anharmonicity and radial coupling is to smear the sideband transition toward the carrier. Following the treatment of [129], Fig. 2.8 also includes a fit to the sidebands. The result of a least-squares fit gave the radial temperature  $T_R$  significantly exceeding the longitudinal temperature  $T_L$ , which is both surprising and in conflict with other measurements. Fortunately, the sidebands remain well-resolved from the carrier transition, so the smearing effects mentioned do not degrade the clock operation.

#### 2.2.4.3 Tunneling and its effects

Tunneling is an effect seen in many quantum systems with periodic potentials, including atoms in optical lattices. As was pointed out in [131], optical lattice clocks with very shallow traps could suffer from residual Doppler and recoil effects (both shifts and line broadening) due to high tunneling rates.

To consider the tunneling rate, we can rewrite the Schrodinger equation for a (1D) lattice potential in the canonical Mathieu form, for which a set of characteristics values  $a_n$  and  $b_n$  correspond to even and odd analytic solutions. These values can then be used to determine the band structure, including the tunneling rate [130]. Fig. 2.9 shows the tunneling rate for the 11 bound



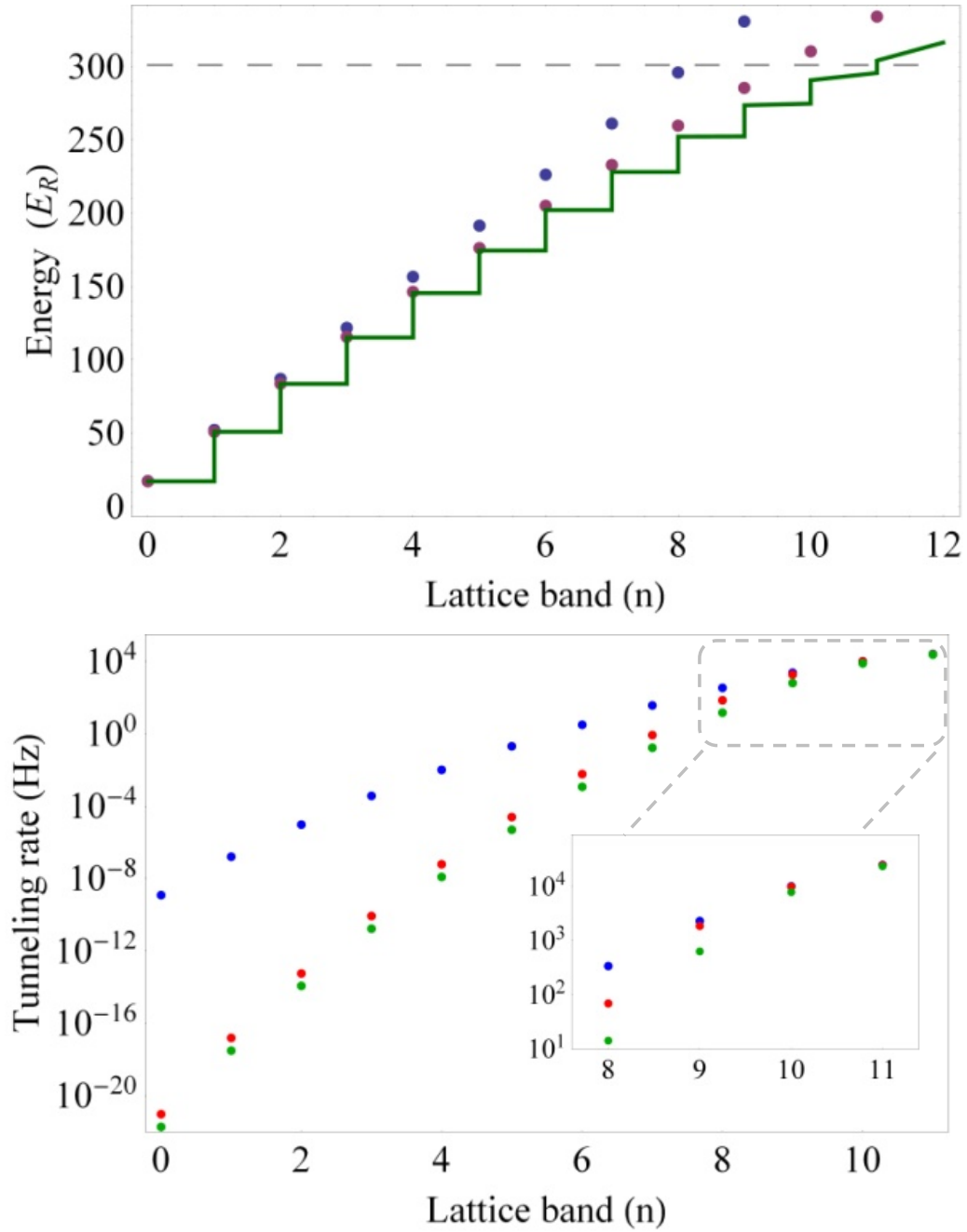


Figure 2.9: Top: Bound states for a  $300 E_r$  lattice. Blue points give pure harmonic oscillator states; purple points are calculated from first-order perturbation theory with a quartic distortion to the harmonic potential; and the green dispersion diagram is the solution to the Mathieu equation. Bottom: calculated tunneling rates for each band. Blue: 1D horizontal lattice (no energy offset). Red: 1D vertical lattice ( $\Delta = 1.6$  kHz due to gravity). Green: 2D lattice ( $\Delta = 2$  kHz due to Gaussian beam). An inset shows the four highest bands at higher resolution.

states of a 300  $E_r$  lattice. On a spectroscopic timescale of 100 ms, only the highest 5 or so bands have non-negligible tunneling rates. However, the rate can become quite large for the highest states (upwards of 10 kHz). Fortunately, very few atoms occupy these states.

One way to suppress tunneling is to introduce an energy offset between neighboring sites. A vertically-oriented 1D lattice accomplishes this via gravity (energy offset  $\Delta = m g \lambda / 2h \simeq 1.6$  kHz, with  $g = 9.8$  m/s<sup>2</sup> the acceleration due to gravity). In the 2D lattice, the Gaussian beam profile associated with the opposite lattice direction also provides an offset ( $\Delta = \frac{1}{2} m \omega_t^2 (\lambda/2)^2 \langle j \rangle = 2$  kHz, with  $\langle j \rangle = 20$  a representative value for the index of the site under consideration).<sup>6</sup> However the energy offset is implemented, the tunneling rate  $J$  in the presence of an energy difference  $\Delta$  becomes  $J^2 / \sqrt{J^2 + \Delta^2}$  [132]. The lower panel of Fig. 2.9 shows that this suppression is most effective for the lower bands but does not vastly improve the situation for the highest two bands.

### 2.3 The role of nuclear spin

Even-mass-number isotopes of alkaline-earth atoms are bosonic and have no nuclear spin. In this case, the clock states are true  $J = 0$ , and the clock transition is highly forbidden. While this makes the clock transition more difficult to efficiently excite, it does have several advantages, including no Zeeman substructure and no dependence upon the lattice polarization (to first order in intensity) [85, 2].

The situation is entirely opposite for odd isotopes: the clock transition is not entirely forbidden, there is Zeeman substructure, and there is some small dependence upon the lattice polarization. All of these effects are due to a non-zero nuclear spin, which perturbs the electronic wavefunctions via the hyperfine interaction.

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<sup>6</sup> Near the center of the Gaussian beam, the energy offset is very small (100 Hz). Away from the center, the Gaussian becomes much steeper, and the energy offset grows. With more than 60 lattice sites between the center of the beam and the edge,  $\langle j \rangle = 20$  is a typical value.

### 2.3.1 State mixing

Following the standard method [133, 134, 135], we can write the four states of an  $nsnp$  configuration in intermediate coupling as follows:

$$\begin{aligned}
 |^3P_0\rangle &= |^3P_0^0\rangle \\
 |^3P_1\rangle &= \alpha|^3P_1^0\rangle + \beta|^1P_1^0\rangle \\
 |^3P_2\rangle &= |^3P_2^0\rangle \\
 |^1P_1\rangle &= \alpha|^1P_1^0\rangle - \beta|^3P_1^0\rangle
 \end{aligned} \tag{2.25}$$

where the superscript “0” denotes a pure  $L - S$  state in the absence of spin-orbit coupling. The mixing coefficients  $\alpha$  and  $\beta$  can be calculated with knowledge of the state lifetimes and energies:

$$\frac{\alpha^2}{\beta^2} = \frac{\tau_{(^3P_1)}}{\tau_{(^1P_1)}} \left( \frac{E_{(^3P_1)}}{E_{(^1P_1)}} \right)^3 \tag{2.26}$$

subject to the normalization constraint  $\alpha^2 + \beta^2 = 1$ . For Yb,  $|\alpha|=0.996$  and  $|\beta|=0.125$ . The  $^3P_1$  state acquires its radiative decay rate to the  $^1S_0$  ground state via this mixing with  $^1P_1$ . The mixing is larger for heavier atoms, producing only a 31 Hz transition width in Mg [94], compared to 182 kHz in Yb and 1.3 MHz in Hg [80].

In odd isotopes with nuclear spin  $I$ , the hyperfine interaction performs additional mixing on states with the same total spin  $F$ . It’s through this mixing that the  $^3P_0$  state gains a finite lifetime and non-zero decay rate to the ground state. The amount of mixing can be calculated from hyperfine and fine-structure splittings and knowledge of the coupling coefficients  $\alpha$  and  $\beta$ . *Porsev, et al.* calculated the  $^3P_0$  lifetime in  $^{171}\text{Yb}$  as 20 seconds, which corresponds to a spectral linewidth of nearly 10 mHz [41]. These numbers are favorable for high-performing clocks, with the lifetime long enough that spontaneous decay is unlikely to limit the observation of narrow atomic spectra, but short enough that the clock transition can be efficiently excited without requiring too much probe light power.

### 2.3.2 Magnetic field sensitivity

As mentioned previously, choosing clock states with  $J = 0$  is beneficial for avoiding polarization-dependent lattice light shifts. A second benefit, though, is that first-order Zeeman shifts are also absent because  $m_J = 0$ . But in the presence of nuclear spin, both clock states acquire total angular momentum equal to the nuclear spin (i.e.  $F = I$ ), which yields  $2I + 1$  substates. For  $^{87}\text{Sr}$ , the only sufficiently abundant odd isotope,  $I = 9/2$ , which creates 10 substates in both the ground and excited clock states, meaning there are 10  $\pi$  ( $\Delta m_F = 0$ ) transitions and 18  $\sigma$  ( $\Delta m_F = \pm 1$ ) transitions [135]! While this doesn't necessarily produce a limitation on the clock's performance, it does add complication. By contrast, Yb is more kind to the experimentalist by offering the simplest fermionic isotope – one with  $I = 1/2$ . Here, there are only two substates in each clock level, two  $\pi$  transitions, and two  $\sigma$  transitions (Fig. 2.10).

There are two sources of Zeeman sensitivity – that arising from the nuclear spin directly, and that arising from hyperfine-induced state mixing. The substates of  $^1S_0$  are affected by the nuclear  $g$ -factor only, while the  $^3P_0$  substates experience both Zeeman effects, for which the total linear Zeeman shift can be written

$$\delta E_B = -(g_I + g_{\text{HFS}}) I_z \mu_B B_z \quad (2.27)$$

with  $\mu_B$  the Bohr magneton and  $B_z$  the magnitude of the magnetic field along  $\hat{z}$ . Note that the above equation adopts the sign convention of Ref. [135]. For  $^{171}\text{Yb}$ ,  $g_I = 0.4919 \mu_N / (I \mu_B) \simeq 5.4 \times 10^{-4}$  [104].  $\mu_N$  is the nuclear magneton, and it is smaller than the Bohr magneton by the ratio of the electron mass to proton mass.

Using the same matrix elements as those used to determine the hyperfine-quenched  $^3P_0$  lifetime, *Porsev, et al.* estimated  $g_{\text{HFS}} \simeq -2.9 \times 10^{-4}$  [41]. However, with Sr it was reported that the relative sign of  $g_{\text{HFS}}$  was opposite from that predicted [135, 40], so the sign requires investigation. The magnitude and sign of  $g_{\text{HFS}}$  can be readily determined by the measuring the splittings between the  $\pi$  and  $\sigma$  transitions, as shown in Fig. 2.10.  $\pi$  transitions are sensitive to  $g_{\text{HFS}}$  only, while  $\sigma$  transitions are sensitive to  $2g_I + g_{\text{HFS}}$ . Experimentally, we found  $g_{\text{HFS}} = +2.73(10) \times 10^{-4}$ , which

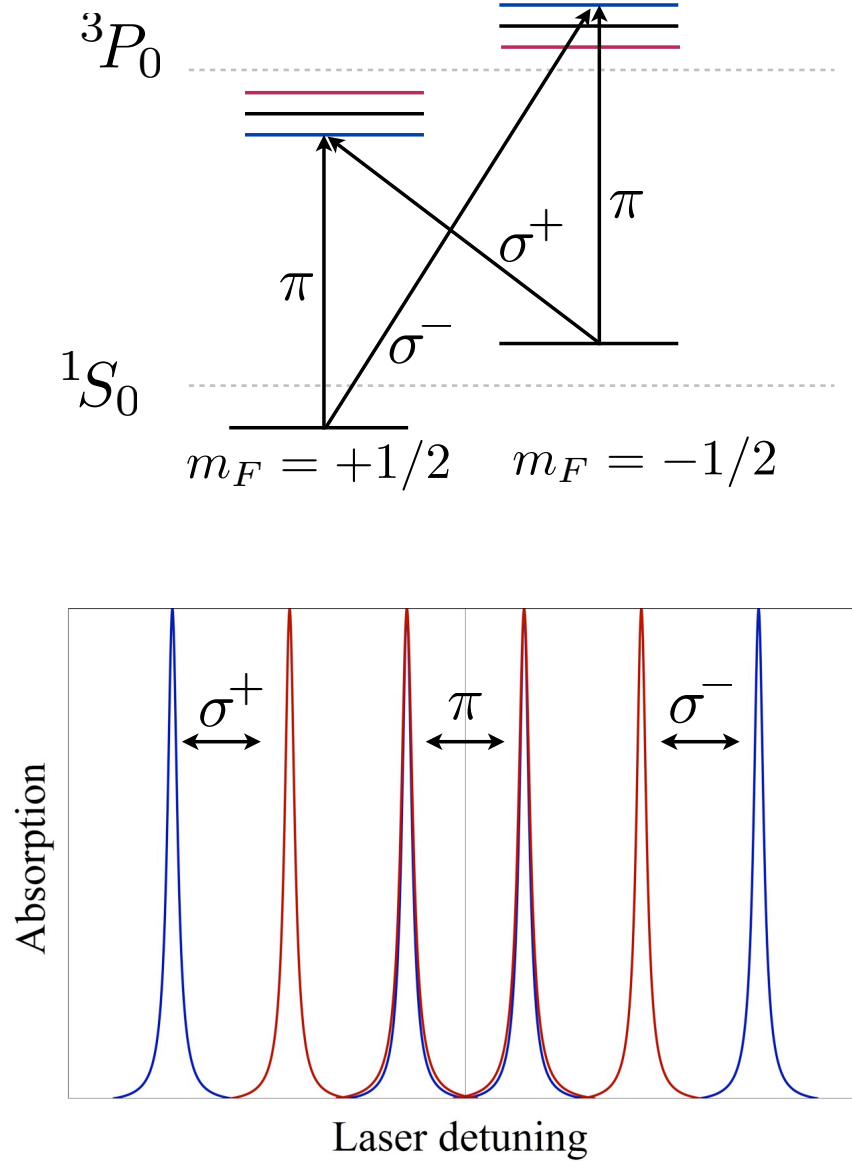


Figure 2.10: Top: Diagram of the Zeeman substructure of a spin-1/2 isotope in a weak magnetic field. The black lines give the  $g$ -factor associated with the nuclear spin. The contribution from hyperfine mixing in  $^3P_0$  is evident in the blue and red lines. Blue corresponds to  $g_{\text{HFS}} > 0$  while red corresponds to  $g_{\text{HFS}} < 0$ . Bottom: The sign of  $g_{\text{HFS}}$  can be determined by examining the absorption spectrum. In either case, the  $\pi$  transitions are the innermost features, but the splitting between the  $\sigma$  transitions is changed depending on the sign of  $g_{\text{HFS}}$ . Experimentally, we found  $g_{\text{HFS}} = +2.55(1) \times 10^{-4}$  for  $^{171}\text{Yb}$ , which most nearly resembles the blue case.

is nearly the magnitude predicted, but indeed with the opposite sign. To state it most explicitly, the hyperfine interaction *increases* the magnitude of the  $^3P_0$   $g$ -factor.

In experimentalist's terms, these sensitivities work out to  $\sim \pm 190$  Hz/G for the  $\pi$  transitions and  $\sim \pm 940$  Hz/G for the  $\sigma$  transitions. One could hope to magnetically shield the atoms to prevent any shift or line broadening, but this could be challenging. A more straightforward technique is to apply a small field (of order 1 G) to cleanly resolve the various transitions, and average over two transitions with opposite dependence (i.e. the two  $\pi$  transitions:  $|m_F = 1/2\rangle \rightarrow |m'_F = 1/2\rangle$  and  $|m_F = -1/2\rangle \rightarrow |m'_F = -1/2\rangle$ ) [136, 89, 1]. Doing so introduces a second-order Zeeman shift which must be calibrated [43]; fortunately, the field can be conveniently monitored by measuring the first-order splitting, from which it is simple to infer the second-order shift.

### 2.3.3 Vector and tensor light shifts

The third effect of nuclear spin is to introduce (via the hyperfine interaction) light shifts which have a dependence on the nuclear spin state  $m_F$ . These so-called vector and tensor polarizabilities (primarily in the  $^3P_0$ ) can interact with the lattice potential to produce polarization-dependent light shifts. The tensor shift arises from the quadrupole part of the hyperfine interaction; the tensor shift for the excited clock state is [135]

$$\delta E_T = \kappa_T U_0 (3 m_F^2 - F(F+1)) \quad (2.28)$$

which vanishes for  $F = 1/2$  [137, 41]. That is, the angular momentum is too small to support a nuclear quadrupole moment. Thus we have found a second advantage to a spin-1/2 isotope such as  $^{171}\text{Yb}$ : there is no need to think any further about tensor shifts to the clock states.

The vector shift is non-zero only in the presence of elliptically-polarized light. To understand this dependence, consider as an example the light shift caused by coupling between  $^3P_0$  and  $^3S_1$ , the latter of which is split into two hyperfine levels,  $F = 1/2$  and  $F = 3/2$ . With linear light, each  $m_F$  state of  $^3P_0$  couples to the same  $m_F$  state in the two hyperfine levels of  $^3S_1$ . However, with circular light (say  $\sigma^+$ ), the  $m_F = 1/2$  state can only couple with one hyperfine level ( $|F = 3/2, m_F = 3/2\rangle$ )

while the  $m_F = -1/2$  can couple with two ( $|F = 1/2, m_F = 1/2\rangle$  and  $|F = 3/2, m_F = 1/2\rangle$ ). This imbalance explains the polarization-dependence of the vector light shift.

The vector shift can be written [41]

$$\Delta\nu_{\text{vs}} = -\frac{m_F}{2F} A \alpha_{\text{vs}} \left(\frac{1}{2}\mathcal{E}\right)^2 \quad (2.29)$$

with  $\alpha_{\text{vs}}$  the vector polarizability at the magic wavelength,  $A$  the degree of elliptical polarization ( $A = 1$  for fully circular and  $A = 0$  for linear polarization), and  $\mathcal{E}$  the electric field of the lattice. Here  $\alpha_{\text{vs}}$  is understood to be that of the  $^3P_0$  only because it is roughly two orders larger than that of  $^1S_0$ . The contribution to  $\alpha_{\text{vs}}$  from a particular intermediate state (e.g.  $^3S_1$ ) can be estimated as the ratio of hyperfine splitting to the detuning [40]. For Yb, a more exact calculation was performed [41], giving  $\alpha_{\text{vs}} \simeq -0.1$  a.u., which is nearly 1600 times smaller than the scalar polarizability. For a trap depth of 1 MHz,  $\Delta\nu_{\text{vs}} \simeq 300$  Hz with a circularly-polarized lattice.

Because of its linear dependence on  $m_F$ , the vector shift can be thought of as a magnetic field aligned along the lattice  $k$  vector. For this reason, one way to suppress the vector shift in a 1D lattice is to orient a real magnetic field perpendicular to  $\vec{k}$ , in which case the two vectors add in quadrature. With this geometry, and with mostly linear polarization ( $A \leq 0.1$ ), the vector shift is already quite small [138, 43]. The effect can be made completely negligible in a 1D lattice by averaging over two transitions ( $m_F \rightarrow m_{F'}$ ) with opposite dependence. However, in higher dimensional lattices, the polarization is more difficult to control, and the geometry suppression may not be possible. In this case, the vector shift could become problematic, as discussed in Sec. 4.4.

## 2.4 Achieving high stability

As mentioned in Ch. 1, one main motivation behind optical clocks is their improved stability over microwave clocks. While the typical stability achieved so far with lattice clocks is far from the fundamental limit, it is still a vast improvement over microwave systems, allowing optical clock measurements to rank among the most precise in all of physics. In this section, we will examine

the two main sources of noise that can degrade the stability of optical lattice clocks.

#### 2.4.1 Quantum projection noise: why more atoms are better

Consider a two-level atom, prepared in a superposition of its eigenstates:  $\psi = c_e|e\rangle + c_g|g\rangle$ . For clock experiments, this state is typically prepared by a nearly-resonant clock pulse, and a measurement of  $c_e$  or  $c_g$  can be used to determine the detuning of the clock light relative to the atomic transition. A well known result of quantum mechanics is that the measurement outcome is not deterministic (except for the trivial case  $c_e = 0$  or  $c_g = 0$ ), but instead has probabilities determined by  $|c_e|^2$  and  $|c_g|^2$ . If one were to repeat this process of state initialization and measurement again and again, it would be clear that the inherent indeterminacy in the measurement causes fluctuations in the outcome and limits a precise determination of  $|c_e|^2$  and  $|c_g|^2$ . This effect has been called “quantum projection noise” because the measurement can be thought of as projecting the atomic state vector onto one of the eigenstates [139]. It is straightforward to show that the increase in precision one gains from measuring  $N$  atoms simultaneously scales as  $\sqrt{N}$  [139, 140] (though advanced techniques may offer a more favorable scaling [141, 142]), and similarly that  $M$  repeated cycles of measurements strung together also increase the precision as  $\sqrt{M}$ .

In normal clock operation, the laser is detuned to alternately probe the half-maximum points of the atomic resonance so as to create an error signal with odd symmetry. For a fraction of atoms excited  $p$  ( $0 < p < 1$ ), the signal-to-noise ratio associated with quantum projection noise is  $\sqrt{N p/(1-p)}$  [139]. One can then write the estimated instability of a projection-noise-limited clock according to the Allan deviation [143] as

$$\sigma_y(\tau) = \frac{1}{\pi Q} \sqrt{\frac{T_c}{\tau} \left( \frac{1-p}{pN} \right)} \quad (2.30)$$

with  $\tau$  the timescale of interest,  $T_c$  the cycle time for each atomic state measurement, and  $Q = \nu_0/\Delta\nu$  the resonance quality factor. The above equation shows both the  $\sqrt{N}$  scaling and the  $\sqrt{M} = \sqrt{\tau/T_c}$  scaling expected.

Even modest parameters suggest  $\sigma_y$  can be quite small in lattice clocks. For  $N = 1 \times 10^4$ ,



$p = 0.4$ ,  $T_c = 1$  s, and  $\Delta\nu = 10$  Hz, then  $\sigma_y(1 \text{ s}) \sim 8 \times 10^{-17}$ . However, the actual instability achieved by lattice clocks is some 20 to 100 times larger (less stable). Clearly some other noise process is playing a role. Two other options related to the measurement of the atomic state are photon shot noise and atom number fluctuations. Together with projection noise, these three terms comprise the “amplitude noise” of the atomic clock.

For any experiment that uses a strong transition to scatter photons off the atoms, as is the case here (see Sec. 3.4), generally each atom has the opportunity to scatter many photons – 1000 or more – during the detection time. Even with poor collection efficiency (due to quantum efficiency in the detector and limited solid angle for photon collection), it’s straightforward to detect more than one photon per atom. In this case, the photon shot noise is lower than the projection noise [140].

Atom number fluctuations, on the other hand, can easily degrade the stability, since the number of photons collected is a function of both the number of atoms in the trap and the detuning of the clock field, and one cannot separate the two contributions with a single measurement. However, a normalized detection technique (again see Sec. 3.4) collects photons from both the ground and excited states, allowing one to divide out any dependence on the atom number and use the calculated signal purely for frequency discrimination [140].

So it seems that amplitude noise does not currently limit the lattice clock. In the next section, we consider frequency noise (specifically that of the local oscillator) and calculate its contribution to the clock stability.

#### 2.4.2 The Dick effect: why dead time can be haunting

Frequency noise on the local oscillator (LO) used to probe an atomic transition can have numerous effects on the resulting spectra. For one, it can lead to imperfect coherence during the light-matter interaction, resulting in broader spectra and/or reduced spectral contrast. Even for a given spectral feature to which one references the LO, fluctuations in the LO frequency lead directly to fluctuations on the clock output *unless* there is sufficient loop gain at the corresponding

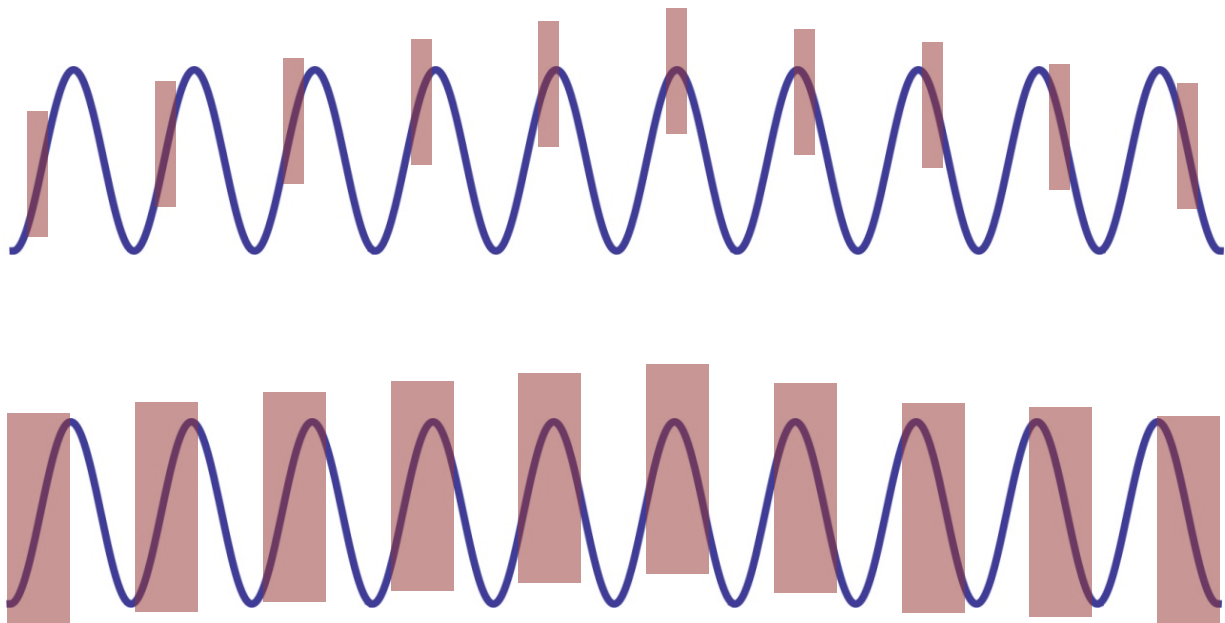


Figure 2.11: Depiction of the downsampling of LO noise that causes the Dick effect. Here, the blue sine wave represents noise at a particular frequency very near the cycle frequency. In the top portion, a small sampling window leads to a larger amplitude of the downsampled noise (evident as the periodic rise and fall of the red boxes). In the lower portion, the sampling window is increased, leading to a reduced amplitude of the downsampled noise (i.e. the red boxes do not rise or fall as much).

Fourier component. Of course, for noise processes faster than the cycle time of the atoms, there's no hope of using the atomic system to eat away the LO noise; it's only for Fourier components slower than the cycle time that the atoms can prevent the LO noise from finding its way onto the total clock signal. Still, this all sounds good so far: provided we're willing to only make frequency measurements on the timescale of a few seconds or slower, the noise properties of the clock should be given entirely by the noise properties of the atoms.

Unfortunately, there's one other hindrance – suppose that we cannot continuously monitor the frequency discriminator provided by the atoms. This is necessarily the case for trapped atom experiments, in which some time must be spent trapping the sample before clock spectroscopy, and further time must be spent detecting the atomic state after spectroscopy. In this case, the atoms are insensitive to frequency excursions of the LO for some fraction of the cycle (the “dead time”). Moreover, the times of high sensitivity (which we want) occur at regularly spaced intervals, as the atoms stroboscopically measure the frequency properties of the LO. For Fourier components on the LO frequency that occur either much faster or much slower than the cycle time, there's no real problem. But for Fourier components very near the cycle time, the stroboscopic measurement will downsample this noise to an even lower frequency, and the clock output will fluctuate. Fig. 2.11 provides one way of viewing this aliasing and downsampling process. The red boxes are successive measurement windows, while the blue curve shows just one of the Fourier components of the LO, one which happens to be very close to the repetition rate of the experimental cycle. For small measurement windows, the average value of the sine wave fluctuates from shot to shot (seen by the slow rise and fall of the red boxes), while for larger windows (bottom of Fig. 2.11) the effect is reduced. Of course, with a duty cycle of unity, one full wave of the sine function can be observed, and it averages to zero.

We can examine this effect – which is generally referred to as the Dick effect [144, 66, 145] – more quantitatively as follows. First, we must define some periodic function ( $g(t)$ ) that summarizes the atomic system's sensitivity to LO fluctuations. Commonly called the sensitivity function,  $g(t)$  depends on the amount of dead time in the cycle and on the type of spectroscopy use (e.g. Ramsey

or Rabi). For the Ramsey case (two pulses of duration  $\tau_p$  separated by the dark time  $T$ , Rabi frequency  $\Omega$ , and with the typical choice  $\Omega \tau_p = \pi/2$ ) we can write [66]

$$g(t) = \begin{cases} a \sin(\Omega t) & 0 \leq t \leq \tau_p & \text{First pulse} \\ a & \tau_p \leq t \leq \tau_p + T & \text{Dark time} \\ a \sin(\Omega [T + 2\tau_p - t]) & T + \tau_p \leq t \leq T + 2\tau_p & \text{Second pulse} \\ 0 & T + 2\tau_p \leq t \leq T_c & \text{Dead time} \end{cases} \quad (2.31)$$

with  $a = -\sin(\delta T)$  with  $\delta$  the LO detuning. Fig. 2.12 shows  $g(t)$  for both the Ramsey and Rabi cases.

Armed with this definition of  $g(t)$ , we can now describe the frequency degradation due to periodic sampling of the LO by again considering the Allan deviation:

$$\sigma_y(\tau) = \left( \frac{1}{\tau} \sum_{m=1}^{\infty} \left( \frac{gc_m^2}{g_0^2} + \frac{gs_m^2}{g_0^2} \right) S_y^f \left( \frac{m}{T_c} \right) \right)^{1/2}. \quad (2.32)$$

Here,  $S_y^f$  is the single-side power spectral density of the fractional frequency fluctuations of the LO at the  $m^{\text{th}}$  harmonic of the cycle frequency  $1/T_c$ . The coefficients  $gs_m$  and  $gc_m$  are the sine and cosine harmonics of  $g(t)$ , defined as

$$\begin{aligned} gc_m &= \frac{1}{T_c} \int_0^{T_c} g(x) \cos(2\pi m x / T_c) dx \\ gs_m &= \frac{1}{T_c} \int_0^{T_c} g(x) \sin(2\pi m x / T_c) dx \\ g_0 &= \frac{1}{T_c} \int_0^{T_c} g(x) dx \end{aligned} \quad (2.33)$$

Together, Eqs. 2.31-2.33 can be used to calculate the Dick effect for a given set of experimental parameters and a known LO noise spectrum ( $S_y^f$ ). We'll revisit these calculations for several sets of parameters in Sec. 3.6, but for now we can instead take the result of Ref. [1] as an example. With state-of-the-art laser stabilization [45], the fractional LO noise is on the order of  $1 \times 10^{-15}$  at timescales from one to a few experimental cycles. A cycle time near 1 s and a interrogation time

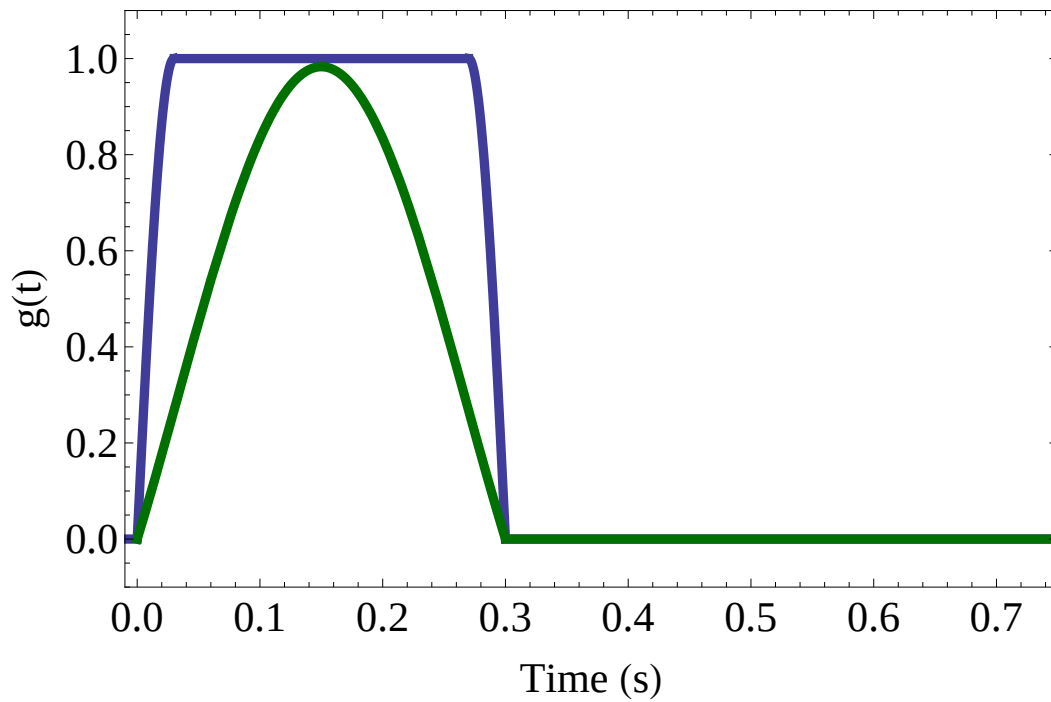


Figure 2.12: Sensitivity function  $g(t)$  for Ramsey (blue) and Rabi (green) interrogation. For both cases, the interrogation time is 300 ms and the cycle time 750 ms. The Ramsey scheme is superior, though, because the short pulses permit a more constant sensitivity.

of 80 ms yield a Dick effect limit near  $\sigma_y$  of  $\sim 2 \times 10^{-15}/\sqrt{\tau}$ . While this result remains among the best stabilities demonstrated to date for any type of atomic clock, it also demonstrates the negative effects of aliasing and downsampling in atomic clocks. Because the Dick effect is significantly larger than the typical value for projection noise, the Dick effect is often the leading noise contributor in optical lattice clocks.

## Chapter 3

### Experimental Details of the NIST Yb Lattice Clock

This chapter gives an overview of the ytterbium clock apparatus, with special attention paid to the elements which have been added or modified since the most recent detailed report [92]. These include a new 399 nm laser system (Sec. 3.1), the addition of a 2D lattice (Sec. 3.2), a spin-polarization technique for  $^{171}\text{Yb}$  (Sec. 3.3), improvements to the detection signal-to-noise (Sec. 3.4), and implementation of higher-performing optical cavities to which the clock laser is referenced (Sec. 3.5), resulting in improvements to the clock stability (Sec. 3.6).

#### 3.1 Two-stage laser cooling

Ytterbium offers two laser-cooling transitions (recall Fig. 1.1): a dipole-allowed transition near 399 nm, and a weaker intercombination (i.e. spin-suppressed) transition near 556 nm. While some experiments have shown success trapping only with the latter transition (and typically using the former for Zeeman slowing [146]), we use both colors for trapping. The 399 nm light is used to collect hot atoms and cool them to a temperature near 1 mK; however, the Doppler limit for this 28 MHz transition (i.e. the heating caused by random photon scattering) prevents reaching ultracold temperatures. Subsequent cooling with the 556 nm light, for which the Doppler limit is 4.4  $\mu\text{K}$ , further reduces the atomic temperature to a few tens of  $\mu\text{K}$ , cold enough for trapping in the lattice.

Early work on the Yb clock at NIST generated the 399 nm light directly with blue diode lasers [75, 92]. These laser diodes were typically centered at a longer wavelength above 400 nm,

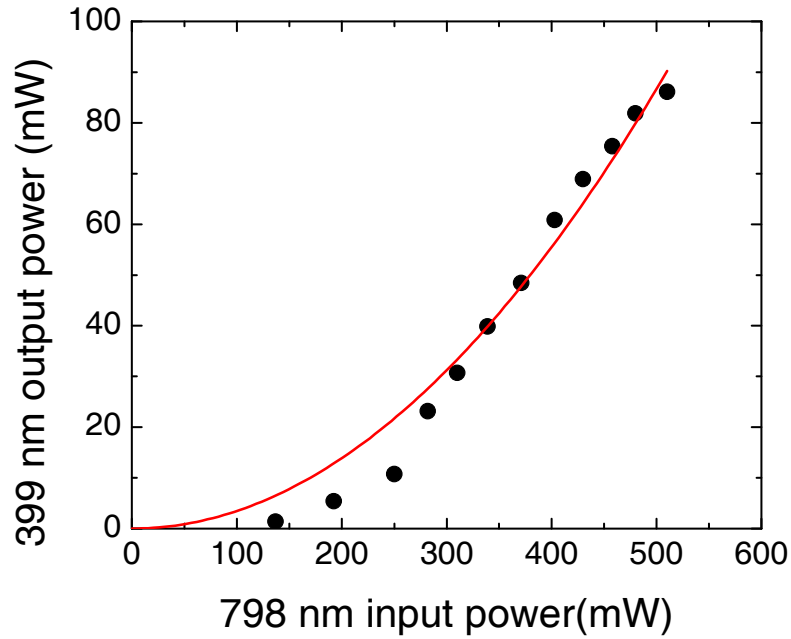
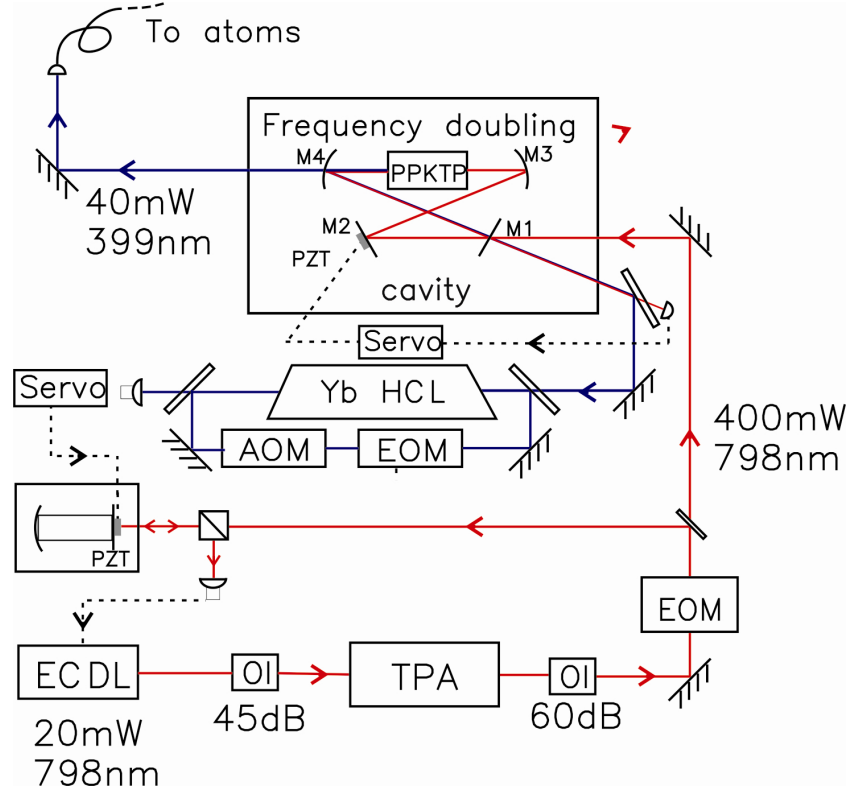


Figure 3.1: Top: Diagram of the 399 nm laser source. Note that OI stands for optical isolator, while other acronyms are defined in the main text. Bottom: Generated 399 nm power as a function of fundamental power.



but with wavelength selection (to identify the diodes that had gain at shorter wavelengths), it was possible to reach 399 nm. Typically three lasers were used simultaneously: one “master” external cavity diode laser (ECDL) [147, 148, 149, 150] that was referenced to an absorption spectrometer, and two “slaves” that were optically injection-locked by the master. This system had several advantages, most notably that it was low-cost and easy to use. However, it also possessed several disadvantages. For one, we were not able to significantly reduce the frequency noise on the master laser when locking it to an optical cavity.<sup>1</sup> Secondly, the AR-coating that was applied to the front facet of the diode was found to degrade over a few months’ time, which made the wavelength of the lasers more difficult to control. Finally, replacement diodes became harder to find, especially once the Blue-Ray wavelength of 405 nm became standard.

We have since implemented an improved 399 nm light source that produces the blue photons by second harmonic generation (SHG) in a ring build-up cavity (Fig. 3.1). The 798 nm fundamental light is generated by an ECDL that is amplified in a semiconductor tapered amplifier. Both the master diode and the amplifier diode are commercially available from Eagleyard Photonics. The ECDL is arranged in a Littman-Metcalf configuration [149, 148], in which the first-order diffraction from a grating is retro-reflected, diffracts a second time, and re-enters the diode. The zeroth-order (undiffracted) light is taken as the laser output; the advantage of this configuration is that wavelength tuning (which is accomplished by tilting the retro mirror) does not steer the output beam. The ECDL output ( $\sim 20$  mW at 798 nm) seeds the tapered amplifier, which typically produces 400 mW of optical power. The majority of this light is used for SHG, though a small portion is split off for wavelength monitoring and for locking the ECDL to a reference cavity via the Pound-Drever-Hall technique [151, 148]. This lock is accomplished with fast electronic feedback to the diode current and with slow electronic feedback to a piezo-electric transducer (PZT) on the retro-reflecting mirror. The cavity has a finesse of about 200, resulting in a linewidth near 1 MHz.

The PDH technique is also used to correct the doubling cavity length (via a PZT on one

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<sup>1</sup> Even though the cooling transition is quite broad (28 MHz), the frequency noise properties of the 399 nm laser are nonetheless very important because we employ a shelving detection scheme on this transition. See Sec. 3.4.

of the mirrors) to stay resonant with the fundamental light. The cavity's input coupler (M1 in Fig. 3.1) is a flat mirror with 99.5 % reflectivity at 798 nm; mirrors M2 (flat) and M3 (15 cm radius of curvature (ROC)) are high reflectors; the final mirror, M4, (15 cm ROC) is a high reflector for 798 nm but transmits the generated 399 nm light out of the cavity. A periodically-poled KTP crystal (1 mm  $\times$  2 mm  $\times$  20 mm) produces the 399 nm light, and is placed between M3 and M4. The cavity is capable of producing as much as 80 mW at 399 nm (Fig. 3.1); a more typical number for day-to-day operation is 40 mW. We have observed temporary degradation effects in the PPKTP crystal, causing the generated power to drop on the timescale of a few hours. This degradation could be due to photorefractive damage [152]. Fortunately, a fairly simple solution is to move the beam to a different spot in the crystal, restoring the power. With good alignment of the doubling cavity, the mode quality of the 399 nm light is sufficiently pure for coupling to a single-mode optical fiber with over 50 % efficiency.

A small fraction of the 399 nm light is reflected by M4 and leaks out M1, overlapped with the prompt reflection of the 798 nm input light. We split the two colors with a dichroic and use the two beams as follows: the 798 nm light is photodetected, forming an error signal for cavity length corrections as mentioned above; and the 399 nm light is sent to a saturated absorption spectrometer [105], which operates in the modulation transfer configuration [106]. The spectrometer uses a hollow cathode lamp (filled with ytterbium and neon buffer gas) as an atomic frequency reference. The isotope can be easily selected by tuning across the various features (see [92] for a sample spectrum). Note that for laser cooling of  $^{171}\text{Yb}$ , we employ the  $F = 1/2 \rightarrow F' = 3/2$  hyperfine transition. A chopping AOM (acousto-optic modulator) creates a discriminator slope for locking, and a lock-in amplifier outputs a voltage which steers the reference cavity (via its PZT) to keep the generated blue light on resonance with the  $^1S_0 \rightarrow ^1P_1$  transition in the HCL.

The 556 nm light is produced via SHG of an 1112 nm Yb fiber laser in a frequency conversion waveguide [92]. The fiber laser was purchased from Koheras and can produce up to 1 W of narrow-linewidth power at the desired wavelength, which is mostly predetermined by the fiber Bragg grating, but can be adjusted somewhat with temperature and a piezo element. The waveguide

was produced by HC Photonics and utilizes MgO-doped PPLN for frequency conversion. The high optical intensity inside the waveguide allows for efficient production of green photons in a single-pass; typically, with 120 mW incident on the waveguide, we see 50 mW of infrared light and 10 mW of green light emerging from the waveguide. Thus, the conversion efficiency can be as high as 20 %. A portion of the green light is sent to a high-finesse ULE optical cavity, which is temperature-controlled and kept under vacuum in order to reduce its drift rate. Electronic feedback corrects the frequency excursions of the fiber laser via an external AOM (for fast corrections) and the fiber laser’s PZT (for slow corrections). Slow drifts of the ULE cavity are manually compensated by changing the AOM frequency every few hours.

Both the 399 nm and 556 nm light have AOM’s installed for frequency tuning, optional power stabilization, and fast shuttering; additional extinction is provided by “quiet” optical shutters purchased from Stanford Research Systems. Optical fibers carry the 399 nm and 556 nm light to the ytterbium apparatus, where each color is split into three beams that are nearly (but not quite) mutually orthogonal. Approximately 5-10 mW of 399 nm light emerge from the fiber, while only 1-2 mW are needed at 556 nm. The three beams at each wavelength, together with their retroreflections, perform six-beam laser cooling in the standard way [12, 153]. An additional fiber carries 5-10 mW of 399 nm light used as a slowing beam that opposes the atomic beam emerging from a small opening in a 450°C oven.<sup>2</sup> The atomic beam is collimated by passing through an aperture (few milli-meter diameter) downstream that also serves as a vacuum conductance limiter, which separates the (higher-pressure) oven region from the (lower-pressure) vacuum chamber. The octagon-shaped chamber has numerous optical viewports, and is maintained (just) below  $10^{-8}$  Torr by a 40 L/s ion pump. The viewport opposite the oven is heated to 300° C and made of sapphire to reduce the rate at which ytterbium deposits onto the viewport, which decreases the optical throughput.

Current-carrying coils are attached to the top and bottom viewports with opposite hand-

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<sup>2</sup> To keep the experiment simple, and to minimize the total beam length, a true Zeeman slower is bypassed in favor of a single slowing beam.

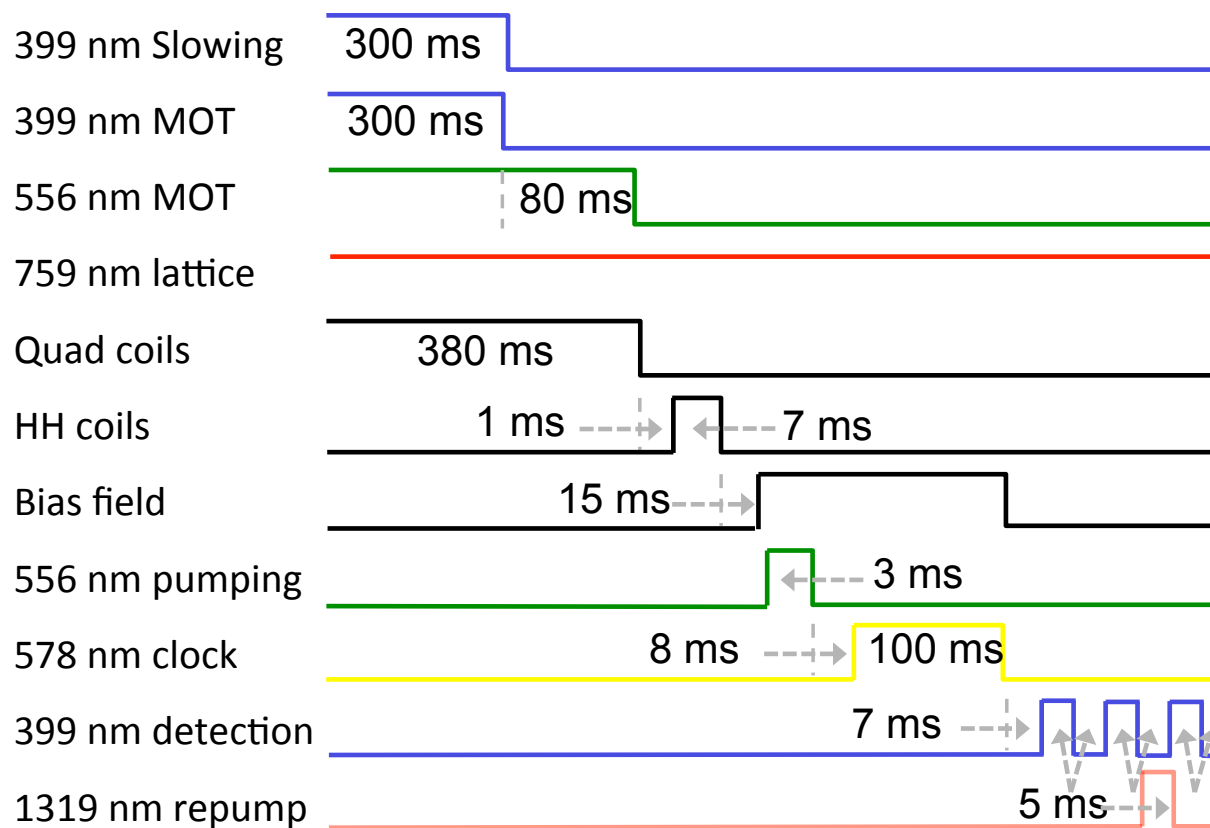


Figure 3.2: Timing diagram for the Yb apparatus.

edness to create a quadrupole magnetic field; these water-cooled “quad coils” carry up to 100 A to create a magnetic field gradient of several tens of Gauss per centimeter. This magnetic field, together with the laser cooling light, creates magneto-optical traps (MOTs) at the two colors. Fig. 3.2 shows a typical timing sequence, with 300 ms devoted to 399 nm cooling, followed by 80 ms of 556 nm cooling. The transfer efficiency from the initial 399 nm MOT to the 556 nm MOT exceeds 50 %. The 80 ms of 556 nm cooling is actually split into three phases, each with a unique optical power, laser detuning, and magnetic field gradient. As the cooling progresses, the optical power and detuning are decreased, while the magnetic field is increased (relative to the first stage of 556 nm cooling, but still below the level used during the initial 399 nm cooling) in hopes of compacting the MOT to be as small as possible. In the end, we have a ball of approximately half a million Yb atoms with temperature  $T_{\text{MOT}} \approx 25 \mu\text{K}$ , ready for loading into the optical lattice.

## 3.2 Lattice trapping

### 3.2.1 Loading atoms in a 1D lattice

The lattice light is produced by an injection-locked titanium:sapphire (Ti:S) laser [154, 92]. The seed laser is an ECDL in the Littman-Metcalf configuration, tuned near the magic wavelength of 759.4 nm, and its output ( $\approx 25$  mW) enters the Ti:S cavity. Electronic feedback to the diode laser current and PZT hold its frequency on resonance with one of the longitudinal modes of the Ti:S cavity. This ring cavity is formed simply by four mirrors and a Ti:S crystal, which is pumped with an 8 W Verdi laser (Coherent, Inc.) at 532 nm. Left unseeded, the Ti:S laser produces 1.6 W of multimode light; with the diode laser seed, the power is the same, but is compressed into a single longitudinal mode.

The center frequency of the lattice light needs to be controlled only at the  $\sim 1$  MHz level, since our current knowledge of the magic frequency has a 10 MHz error bar (see Ch. 4). However, this is still somewhat difficult, since there is no nearby resonance in Yb to which we can reference. For initial measurements, the frequency of the Ti:S laser was actively locked to the frequency comb

via slow feedback to an intra-cavity PZT [126]. More recently, we have instead locked the Ti:S laser to a small ULE cavity. The cavity has medium-high finesse at 759 nm, and it is held at UHV pressure by an ion pump and temperature-controlled to have a low drift rate. Measurements with the frequency comb suggest the drift of this ULE cavity is no more than 10 Hz/s, and the daily drift rate is less than 1 MHz. This drift rate is sufficiently low that we need only to check the Ti:S frequency every few days with a frequency comb and make corrections at the MHz level as needed. Moreover, we have found that the cavity lock actually narrows the noise spectrum of the Ti:S to the level of a 1 kHz linewidth.

After an AOM for intensity control, the output of the Ti:S laser is coupled into a single-mode optical fiber and delivered to the Yb trap. As much as 1 W emerges from the fiber and is collimated to have a large beam size. An achromatic lens (30 cm focal length) focuses the light to a waist  $w_0 \approx 45 \mu\text{m}$  ( $1/e$  field radius). A curved mirror (ROC = 30 cm) retro-reflects and re-focuses the light, steering the light back into the optical fiber. Both the lens and retro-reflector are mounted on translation stages in order to adjust the location of the waist and match it to the position of the 556 nm MOT.

As shown in Fig. 3.2, the lattice laser illuminates the atoms during both stages of laser cooling. This is done for simplicity, and presumably we compensate for the differential Stark shifts on these transitions by adjusting the laser detuning for maximum atom number. After the 80 ms of cooling on the 556 nm transitions, all light sources (excluding the lattice) are extinguished, along with the quadrupole magnetic field, and approximately 3 % of the MOT atoms are trapped in the lattice. Because the lattice depth (30-50  $\mu\text{K}$ ) is only a little higher than the atomic temperature, some of the loss in atoms can be attributed to temperature. However, we speculate that a larger effect is that the lattice waist (45  $\mu\text{m}$ ) is smaller than the MOT radius (180  $\mu\text{m}$ ). Thus, a larger beam could potentially trap many more atoms; however, to achieve the same trap depth would then require much more optical power, which could only be achieved with a buildup cavity. We have plans to install such a buildup cavity in the future, but for now, the number of atoms trapped in the 1D lattice is of order 25,000, which is more than enough to produce a high signal-to-noise

ratio. This corresponds to an estimated density of  $3 \times 10^{11}/\text{cm}^3$  (see Appendix A.1 for details).

The atomic temperature along the lattice direction can be determined by sideband spectroscopy. We typically see temperatures between 8 and 15  $\mu\text{K}$ , which is a little colder than the MOT temperature, confirming that slower atoms are more likely to be trapped by the lattice. We have also measured the transverse temperature by probing the atoms orthogonal to the laser direction. In this case, the sideband structure is not resolved, and we see a lineshape resembling a Gaussian (though a bit asymmetric). A Gaussian fit reveals the temperature as in Eq. 2.2; typically, we find the longitudinal and transverse temperatures to be the same, within 20 %.

We can also measure the lifetime of atoms in the lattice by monitoring the atom number over time. Typically, we find the  $1/e$  lifetime to be 300–500 ms. We have measured the lifetime at several different trap depths to see if photon scattering played a role; no dependence was observed. We also, for a brief time, had a shutter installed between the oven and the chamber, allowing us to block the atomic beam after the lattice was loaded.<sup>3</sup> We checked to see if blocking the atomic beam increased the lattice lifetime, but again no dependence was observed. We thus conclude that the lattice lifetime is limited by the relatively high background pressure ( $5\text{--}10 \times 10^{-9}$ ). Studies with a similar apparatus have shown that the residual gas is predominantly hydrogen, and that the pressure can be substantially reduced (by a factor of ten or more) by adding more pumping speed and by narrowing the differential pumping tube. The 400 ms lifetime is long enough that it does not limit normal clock operation; however, when trying to achieve the narrowest atomic spectra (which require the longest probe times), we had difficulty retaining enough atoms to keep the signal-to-noise ratio high (see Sec. 3.6 below).

### 3.2.2 Loading a 2D lattice

For most measurements, a 1D lattice provides sufficient confinement, but there are potential advantages to higher-dimensional confinement. In particular, a 2D lattice was a very useful tool

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<sup>3</sup> Unfortunately, the shutter overheated and stopped functioning. Even worse, it was in the closed position, forcing us to break vacuum and remove the shutter.

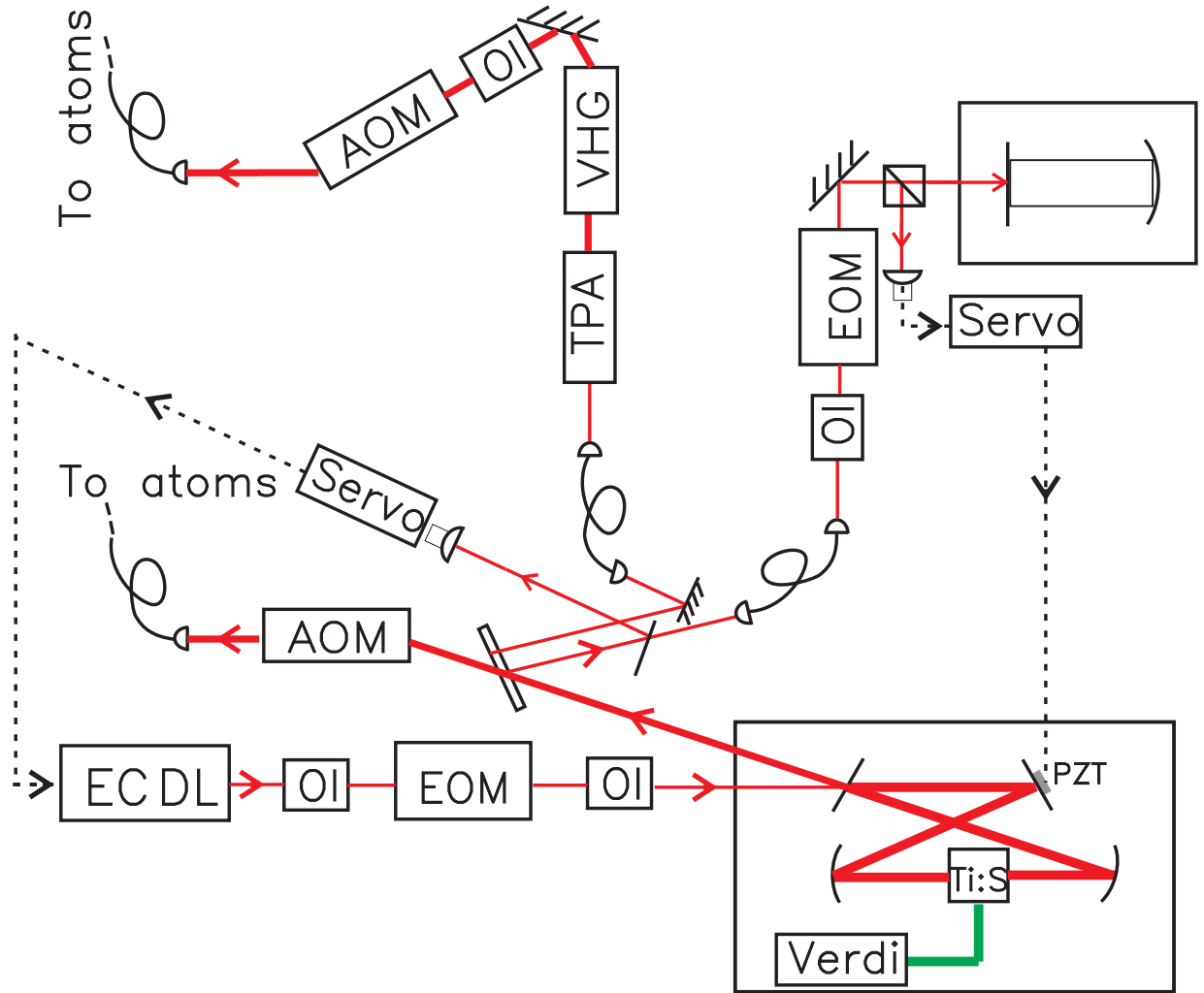


Figure 3.3: Diagram of the lasers used to form the 2D lattice. An external cavity diode laser (EC DL) is locked to the Ti:Sapphire laser cavity via the PDH technique, with feedback to the diode laser current and PZT. The diode light then optically seeds the Ti:S laser, which is pumped with an 8 W Verdi laser. The majority of the Ti:S output passes through an AOM for intensity control, before being sent to the atoms via optical fiber. A small part of the Ti:S light is sent to a ULE cavity, which serves as the long-term frequency reference. A second pickoff of the Ti:S output seeds a tapered amplifier (TPA). The output of the TPA passes through an optical isolator (OI), volume holographic grating (VHG), and an AOM (for intensity control), before being launched into an optical fiber.



as we investigated the cold collision shift in hopes of understanding and controlling the collisions (Ch. 5). As discussed in Sec. 2.2.2, our 2D lattice is formed from two separate, non-interfering lattices. The optics that form the second lattice are nearly identical to the first: light from a fiber is collimated, then tightly focused, and retro-reflected with a curved mirror. Rather than split the output of the Ti:S laser between the two lattices, we implemented a tapered amplifier to supply the power for the second lattice (Fig. 3.3). A small portion of the Ti:S output is used to seed the TPA so that the two lattices are at the same frequency; however, each has an independent AOM, giving us the flexibility to offset the frequencies of the two lattices, which we do for purposes of suppressing the vector Stark shift (Sec. 4.4). The output of the TPA passes through a volume holographic grating (VHG) to suppress its broad, incoherent background spectrum.

Both lattices illuminate the atoms during the laser cooling stages. After the cooling light is extinguished, the distribution of trapped atoms looks like two crossed 1D lattices, as shown in the left camera image in Fig. 3.4. To form a 2D lattice, we must remove those atoms which are only confined by one of the beams. This is accomplished by slowly turning off the power in one lattice beam (via its AOM), then slowly increasing it back up; the same procedure is then repeated for the other lattice beam. The ramp times and hold times (at zero power) are all 10 ms. We observe that 15 % of the atoms remain after this filtering step, which is roughly consistent with the fraction initially confined in the central overlap region of the two 1D lattices (Fig. 3.4). For typical operating conditions, we estimate that this leads to 7,000 atoms in 25,000 lattice sites, with  $\approx 25$  % of the atoms in doubly-occupied sites (Appendix A.2).

The right camera image in Fig. 3.4 strongly suggests that we have indeed removed the 1D atoms, leaving behind a true 2D sample. To gain further confidence, we employed a modified spectroscopic technique wherein the clock probe beam is tilted with respect to the lattices. While under normal operation, the probe is precisely aligned along the horizontal lattice, here we tilt it by  $\approx 10$  mrad in the vertical direction, so that the beam lies in the plane formed by the two lattices. In the lower panel of Fig. 3.4, we see two scans of the clock transition, with and without the second dimension of confinement. In the 1D lattice (blue points) case, motional sidebands near 300 Hz

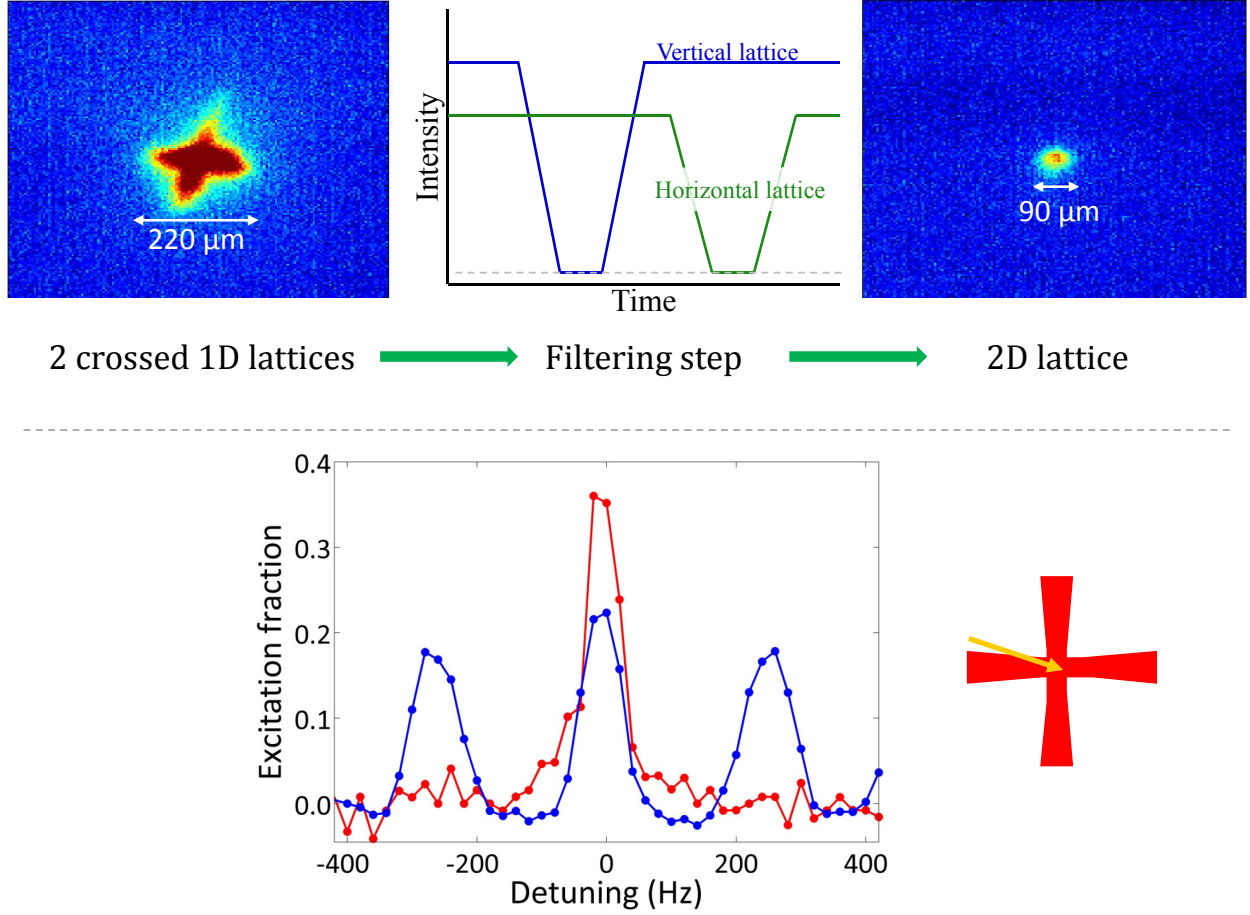


Figure 3.4: Top: Shown are false-color images obtained by collecting 399 nm fluorescence. At the left are two crossed 1D lattices. At the right is the image from a 2D lattice. In between is a diagram of the filtering sequence used to ensure true 2D confinement. Bottom: With the spectroscopic beam tilted with respect to the lattice axis, we see that the transverse motional sidebands in a 1D lattice (blue) are suppressed in a 2D lattice (red).

are clearly visible, while in the 2D case (red points) the sidebands are absent. This result suggests that the filtering procedure yields a true 2D sample.

### 3.3 Spin polarization via optical pumping

With atoms loaded in a 1D or 2D lattice, the next step is to prepare them for spectroscopy. Initially, the population is split between the two spin-states of  $^1S_0$ , which has several consequences. First, assuming we apply a small magnetic field to resolve the various transitions (which we always do), then only half the atoms can be simultaneously excited by the clock laser, which divides the spectral contrast by two. Perhaps more significantly, two atoms in different spin states are not identically-prepared, which prevents using quantum statistics to control their collisional processes. For both these reasons, we have implemented a spin-polarization protocol that employs 556 nm light to pump all the atoms to a single spin-state. Benefitting from the simplicity of a spin-1/2 isotope, this protocol is remarkably simple: the atoms are illuminated with a short pulse of light, tuned to a specific frequency and with a well-defined polarization.

Fig. 3.5 shows a level diagram for this process. Under a uniform magnetic field of 4 G, the substates of  $^3P_1$  are split by 6 MHz/ $m_F$ . A 1 ms pulse with intensity  $\sim 10 \mu\text{W}/\text{cm}^2$  (or about 10 % saturation) drives  $\sigma^+$  and  $\sigma^-$  transitions. The light is chosen to be resonant with either the  $|^1S_0, m_F = -1/2\rangle \rightarrow |^3P_1, m_F = 1/2\rangle$  transition or the  $|^1S_0, m_F = 1/2\rangle \rightarrow |^3P_1, m_F = -1/2\rangle$  transition. The relevant Clebsch-Gordan coefficients dictate that atoms in  $^3P_1$  are more probable to decay on a  $\pi$ -transition (no change in spin state) than a  $\sigma$ -transition, by a factor of two. Those atoms which do decay on a  $\sigma$  transition are returned to their original spin-state, where they can again absorb a 556 nm photon and “try again”; atoms which decay by  $\pi$ -transition remain in their new spin state, from which they cannot be excited again. This is because the 556 nm light has the improper polarization (but the right frequency) to drive  $\pi$ -transitions, and it has the improper frequency (but right polarization) to drive  $\sigma$ -transitions. Of course, neither of these cases is impossible: the wings of this 182 kHz Lorentzian lineshape<sup>4</sup> allow for finite excitation even with

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<sup>4</sup> In fact, the line is likely broadened beyond the natural linewidth by Stark shifts from the lattice light.

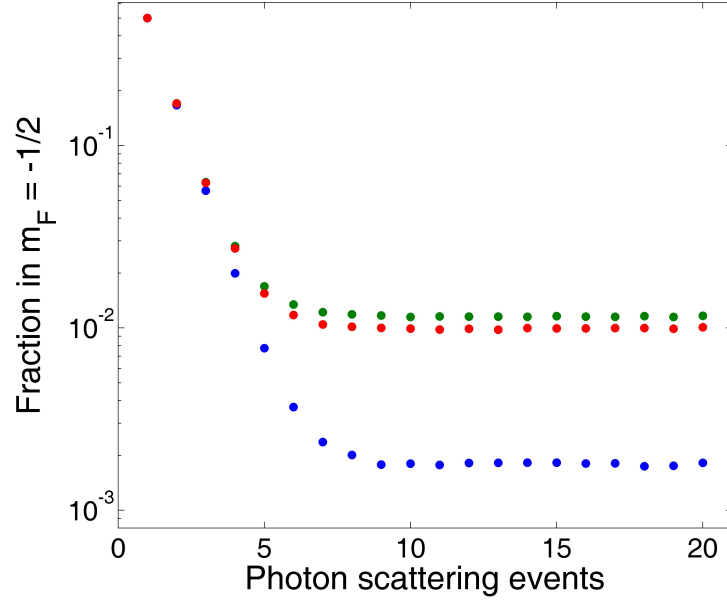
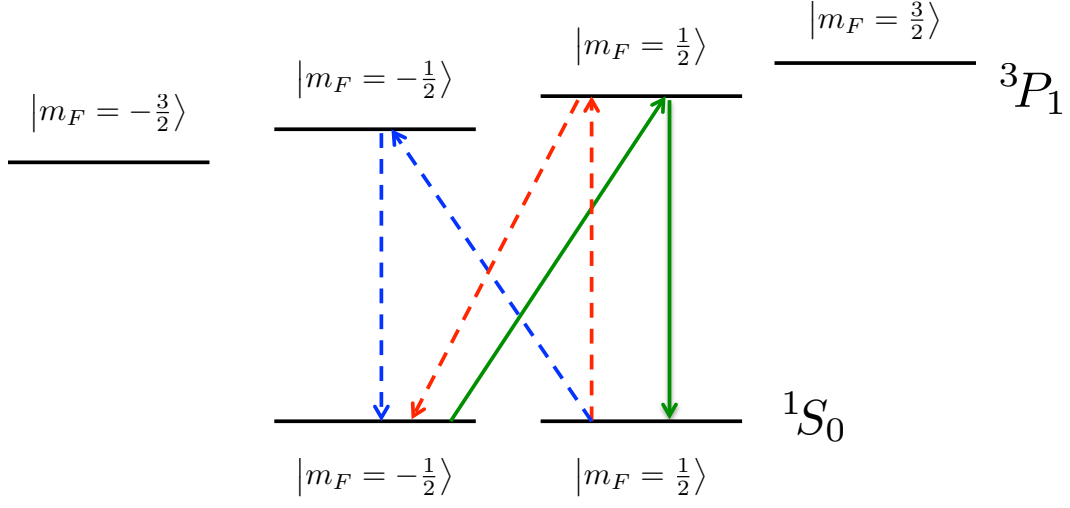


Figure 3.5: Top: Diagram of the optical pumping procedure by which the atoms are spin-polarized to a single ground state of  $^1S_0$ . Shown here (green lines) is the pumping procedure for  $|m_F = -1/2\rangle \rightarrow |m_F = 1/2\rangle$ . Also shown are two processes by which the atoms can “escape”: off-resonant excitation (dashed blue) and imperfect optical polarization (dashed red). Bottom: Monte-Carlo simulation of the pumping process. The population begins as a 50/50 mixture; after a few photon absorption and re-emission events, the population quickly converges to a single spin state, with  $\sim 1\%$  impurity. The blue dots have only the off-resonant excitation escape process (for 6 MHz splitting between the inner states of  $^3P_1$ ); the red dots have only the impure polarization escape procedure (for 1% linear polarization); and the green dots have both processes.

6 MHz splitting, and the optical polarization is impure at some level. The lower panel of Fig. 3.5 shows a Monte-Carlo simulation of this spin-polarization process, including these two “escape” mechanisms that limit the fidelity of the spin-polarization. Experimentally, we routinely observe that level of impurity in the spin-polarization is near 1 % (Fig. 3.6). With the goal of increasing spectral contrast, those few atoms left in the “wrong” spin state offer little improvement; however, from the standpoint of collisional processes, it could be that the spectator atoms in the opposite spin-state cause significant collision shifts. This was investigated (Ch. 5), and it was ultimately found that they do not play an important role.

In order to obtain this low level of impurity, it is necessary to control the magnetic field environment, including both the decaying quadrupole magnetic field (used during the MOT) and the static stray field seen by the atoms. The latter is readily canceled using three pairs of small current-carrying coils (one for each direction), and by monitoring the splittings of the various  $m_F$  states of  $^3P_1$  we can zero out the magnetic field to within 10 mG. However, the decaying magnetic field from the MOT coils is a bit trickier. While the current in the MOT coils can be shut off quickly ( $< 1$  ms), we have found that the actual magnetic field takes longer to decay, presumably because of induced currents in the surrounding metal apparatus. Using  $^3P_1$  spectroscopy at various wait times after the MOT, we mapped out the magnetic field decay, and found it was exponential, with a  $1/e$  decay time of 12(2) ms and initial value (immediately after the green MOT) of 2 G; thus, to reach residual fields below 10 mG requires waiting 70 ms, which is longer than we care to wait. Instead, we implemented a conditioning step as follows: 1 ms after the current is extinguished in the quadrupole coils, we flip the direction of one coil (via solid-state relays) to produce a Helmholtz geometry [2, 92]; a subsequent burst of current (several tens of amps) is turned on for 7 ms. With this conditioning trick, we observe a  $1/e$  decay time near 1 ms, a factor of ten improvement. After 15 ms of wait time, we proceed with the spin-polarization as described above.

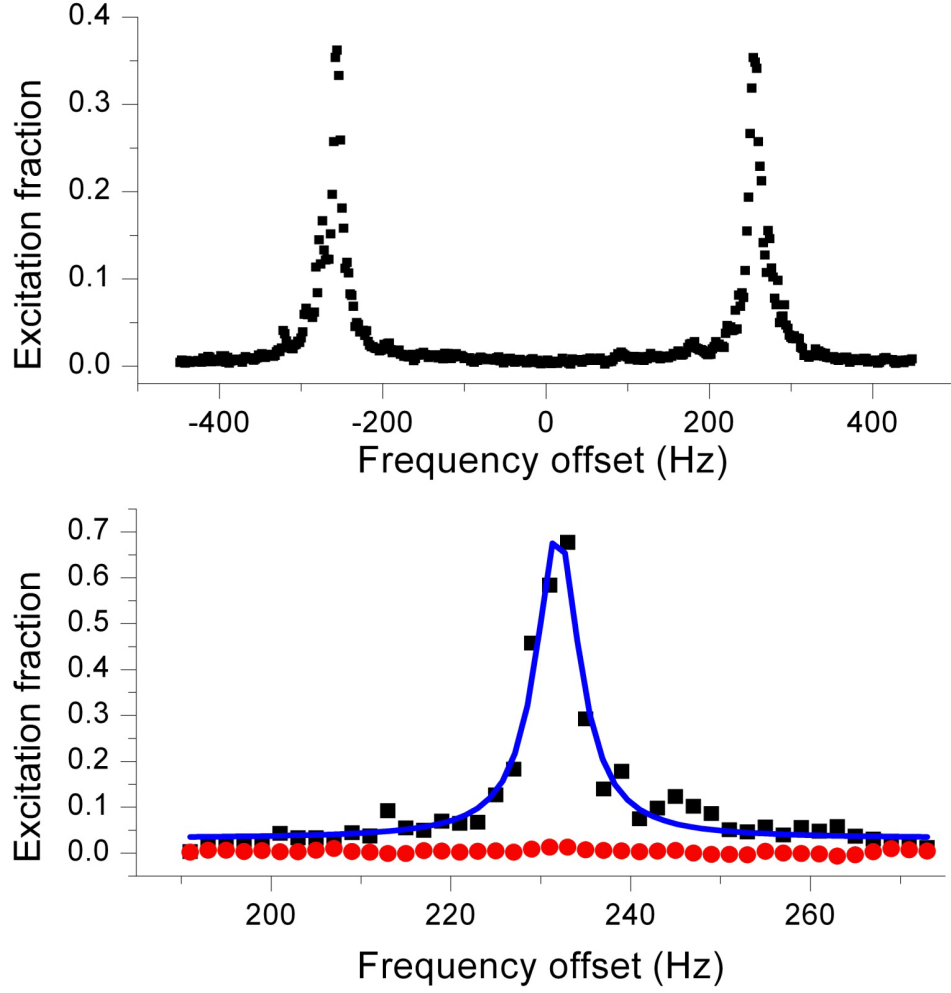


Figure 3.6: Top: Spectrum of the  $\pi$  transitions in  $^{171}\text{Yb}$  with a small bias magnetic field. Bottom: Zoom in on the  $m_F = -1/2$  transition, with atoms optically pumped into (out of) this state shown in black (red) markers. The blue curve is a Lorentzian fit with a FWHM linewidth of 5.5 Hz, consistent with the Fourier limit for a Rabi probe time of 160 ms. These traces were taken before the improved cavity systems were implemented (see Sec. 3.5 below); for that reason, the data are averaged five times to suppress clock laser noise.

### 3.4 Normalized shelving detection

After the atoms have been excited on the clock transition, it is necessary to read out the atomic state by some suitable detection scheme. When considering noise processes which limit the signal-to-noise ratio of this detection (Sec. 2.4), three sources were mentioned: atom number fluctuations, photon shot noise, and quantum projection noise. The projection noise is in many ways the fundamental limit, as it can only be made smaller with more atoms. For lattice clocks, the projection noise limit still corresponds to a large S/N, but reaching that level is not trivial. In this section, we will consider the first two noise sources in the above list, showing that they can indeed be kept smaller than the projection noise, enabling a high signal-to-noise readout of the atomic state.

The detection technique we employ is known as shelving detection, which has a long history in spectroscopy of atoms and ions [155, 156, 157, 158]. The strength of the technique is that it provides the opportunity to query the atom's state many times by repeatedly scattering photons in a suitable cycling transition. For a single atom or ion, this enables an unambiguous determination of the atomic state. This is true even when the detector misses the vast majority of the photons (due to limited collection angle and inefficiency in photodetection) because there either are, or are not, any photons scattered. With an ensemble of atoms, it's the fraction of atoms in a particular state we're after, and photon shot noise and atom number fluctuations can hamper the ability to determine that excitation fraction.

In the Yb experiment, we detect the fraction of excited atoms by applying a sequence of three pulses resonant with the cooling transition at 399 nm and collecting the scattered fluorescence on a photomultiplier tube (PMT). Each PMT signal is integrated and subsequently digitized by a microprocessor (Fig. 3.7). The first pulse measures and heats away all atoms remaining in the ground state after spectroscopy; the second pulse measures the background signal due to fluorescence from the thermal atomic beam; and the third pulse measures the atoms that were excited to the long-lived  $^3P_0$  state by pumping the atoms back to the ground state with the  $^3P_0 \rightarrow ^3D_1$

transition at 1388 nm, which subsequently decays to the ground state via the  $^3P_1$  intercombination transition. From these three signals (ground state population ( $G$ ), excited state population ( $E$ ), background level ( $B$ )) the microprocessor computes a normalized excitation fraction to reduce the effects of shot-to-shot atom number fluctuations. The excitation fraction is

$$F_E = \frac{E - B}{E + G - 2B}. \quad (3.1)$$

The pulse times (5 ms each) are relatively long, leaving plenty of time for the atoms to scatter many photons before being heated out of the trap. In truth, the signal has decayed substantially after 2 ms, so that by the end of the 5 ms, only background fluorescence is collected. The optical power of the 399 nm pulses is controlled by a power servo that feedbacks on an AOM; intensity fluctuations are held well below 1 %. As mentioned above, the newer 399 nm laser source (generated via SHG of 798 nm diode light) has lower frequency noise than its direct-diode predecessor; examining the locked error signal of the 798 nm stabilization cavity suggests frequency excursions below 1 kHz. The 1388 nm light source is a DFB laser, commercially available from ExceLight. We found it was necessary to use several optical isolators to keep this laser well-behaved. Its wavelength is not actively maintained, yet we do not need to tune the laser more than twice per day (and even then, not very far).

The relative noise contribution of shot noise, compared to projection noise, comes down to how many photons are collected per atom. In our geometry, a lens is mounted just outside of one viewport of the vacuum chamber, which is about 40 mm away from the atoms. The solid angle through which photons are collected, compared to the  $4\pi$  into which they are emitted, works out to 4 %. The PMT has a quantum efficiency near 18 %, and these two effects give a combined collection efficiency of 0.7 %. Fortunately, each atom scatters many photons before it is heated from the lattice. With a saturation parameter near 2, the photon scattering rate is approximately 1/3 of the excited state decay rate [153], which here works out to each atom scattering a photon every 17 ns. So in the time of 1 ms (before very many of the atoms have been heated away), we collect something like 400 photons from each atom. Thus, photon shot noise is much smaller than



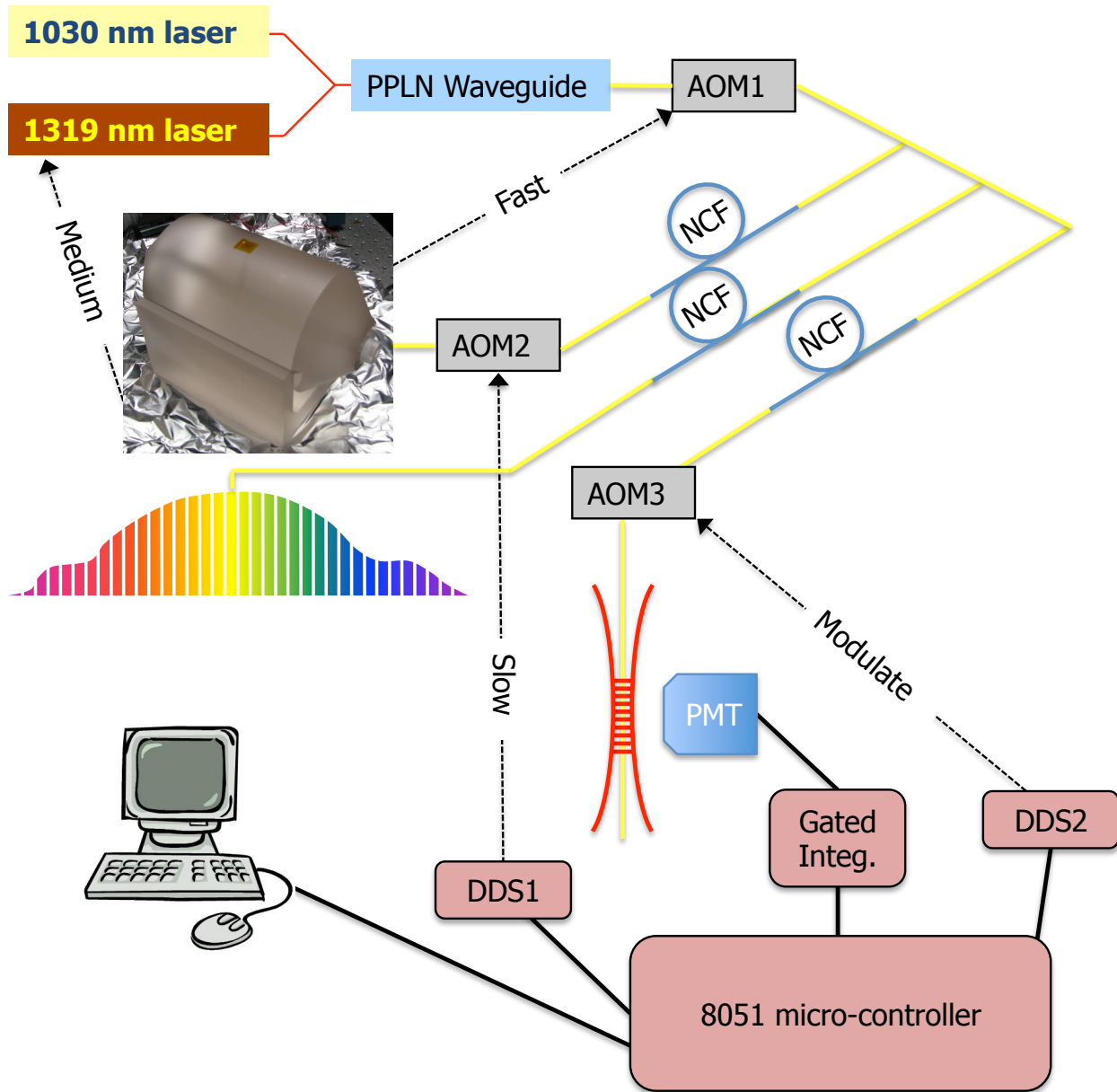


Figure 3.7: Diagram of the clock light distribution and signal processing. The 578 nm clock laser is produced by sum-frequency-generation in a waveguide; the output is split into three paths, one each for the frequency comb, optical lattice trap, and optical cavity, each delivered by its own noise-canceled fiber (NCF). Electronic feedback (shown in the dashed black lines) locks the laser to the optical cavity on fast and medium timescales. After driving the clock transition in the lattice-trapped atoms, a photomultiplier tube (PMT) collects scattered photons from the 399 nm detection pulses as described in the main text; the PMT's output is integrated and digitized. The micro-controller determines the excited fraction and updates two direct digital synthesizers (DDS) in order to lock the clock laser to the center of both nuclear spin transitions. The micro-controller also sends data to a PC (by its serial port) for data-logging and analysis.

quantum projection noise.

Shot-to-shot atom number fluctuations are typically on the level of 10 % of the total atom number, though occasionally they can be larger. Fortunately, the normalization scheme strongly suppresses these fluctuations. We have observed that typically 90 % of the excited atoms are repumped back to  $^1S_0$ , which is nearly consistent with the limit imposed by branching ratio considerations.<sup>5</sup> With the normalization scheme in place, we have seen signal-to-noise ratios between 50 and 150, which are consistent with, or perhaps a factor of 2 smaller than, the projection-noise limit.

### 3.5 Clock laser pre-stabilization

As discussed in Sec. 2.4, the noise properties of the LO (that is, the clock laser) are critical in determining the stability of the clock. State-of-the-art laser stabilization usually involves phase-locking a laser source (with electronic feedback) to a single longitudinal and transverse mode of a passive, ultrastable Fabry-Pérot (FP) cavity. The FP cavity consists of very high-reflectivity mirrors, optically contacted onto a rigid spacer. In the limit of good signal-to-noise ratio and tight phase lock, the length stability of the FP cavity gives the frequency stability of the resulting optical wave. A fundamental limit that many cavity-stabilized lasers have reached is given by Brownian thermal mechanical fluctuations of the FP cavity. This  $1/f$  thermal noise ( $f$  the Fourier frequency) produces a flat Allan deviation, and it is typically dominated by the contribution of the two cavity mirrors (rather than the spacer). In this case, the thermal noise is [160, 161, 46]

$$\sigma_{\text{therm}} = \sqrt{\frac{8 k_B T \ln 2}{\pi^{3/2}} \frac{1 - \sigma^2}{E w_0 L^2} \left( \phi_{\text{sub}} + \phi_{\text{coat}} \frac{2}{\sqrt{\pi}} \frac{1 - 2\sigma}{1 - \sigma} \frac{d}{w_0} \right)}. \quad (3.2)$$

Here,  $\sigma$ ,  $E$  and  $\phi_{\text{sub}}$  are Poisson's ratio, Young's modulus and the mechanical loss for the mirror substrate,  $w_0$  is the laser beam ( $1/e$  field) radius on the mirror,  $T$  is the mirror temperature in Kelvin,  $k_B$  is Boltzmann's constant, and  $L$  is the cavity length.  $\phi_{\text{coat}}$  and  $d$  denote the mechanical

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<sup>5</sup> Assuming  $LS$ -coupling, the branching ratios (including the  $\omega^3$  dependence)  $f_J$  from  $^3D_1$  to  $^3P_J$  are  $f_0 = 0.639$ ,  $f_1 = 0.352$ , and  $f_2 = 0.0094$  for  $J = 0$ ,  $J = 1$ , and  $J = 2$ , respectively [159]. Because atoms that decay to  $^3P_0$  can be excited again by the repumper, the branching-limited repump efficiency is given by  $1 - \frac{f_2}{f_1 + f_2} \approx 97\%$ .

loss and thickness of the thin-film reflective coating. The first term in parentheses is the mirror substrate contribution and the second term is the contribution from the coating. High-stability FP cavities are typically made from ultralow expansion (ULE) glass to reduce cavity length changes due to temperature drift around room temperature. Cavity lengths are often 10–20 cm. Under such conditions, the lowest thermal noise instability is typically between  $3 \times 10^{-16}$  and  $1 \times 10^{-15}$ , roughly consistent with the best experimentally observed instability [162, 163, 45, 164]. The first cavity used on the Yb experiment was of the “football” design [45, 165], for which the thermal noise limit was a bit over  $1 \times 10^{-15}$ . To reduce thermal noise, the choice of mirror substrate material ( $E$  and  $\phi_{\text{sub}}$ ), beam radius ( $w_0$ ), cavity length ( $L$ ) and cavity temperature ( $T$ ) can be modified. Each modification presents different technical challenges. Our approach was to fabricate a long cavity featuring a larger beam size and alternative mirror material.

Because the thermal expansion of the cavity must be controlled well, we chose ULE glass as the cavity spacer material. For the mirrors, however, we chose fused silica, because its value of  $\phi_{\text{sub}}$  is more than ten times smaller than that for ULE [160, 163, 166]. Consequently, the substrate thermal noise term shrinks below that of the thin-film reflective coating (Eq. 3.2, second term in parentheses), and  $\sigma_{\text{therm}}$  is reduced by 1.8. With this modification, the contribution of the thin-film coating dominates, and  $\sigma_{\text{therm}}$  can be further reduced by exploiting its  $1/w_0$  [161, 167] and  $1/L$  dependencies. We therefore chose a long cavity ( $L \approx 29$  cm) with a longer radius of curvature ( $R = 1$  m) for both cavity mirrors, yielding  $w_0 \approx 275 \mu\text{m}$ . With these cavity parameters, we reduced the thermal-noise-limited fractional frequency instability to  $1.4 \times 10^{-16}$ .

In hopes of realizing instabilities as low as this, we constructed two similar cavity systems and measured the laser coherence properties between them. Several milliwatts of laser light at 578 nm were divided into multiple paths, including one for each of the two cavities. Each cavity was enclosed in a vacuum chamber, which was single-stage temperature controlled (fluctuations over 24 hours at a few millikelvin). One important cavity design consideration was the reduction of length changes due to acceleration-induced deformation. We implemented a cavity mounting design similar to those described in [163, 168], with the cavity resting on four symmetrically placed

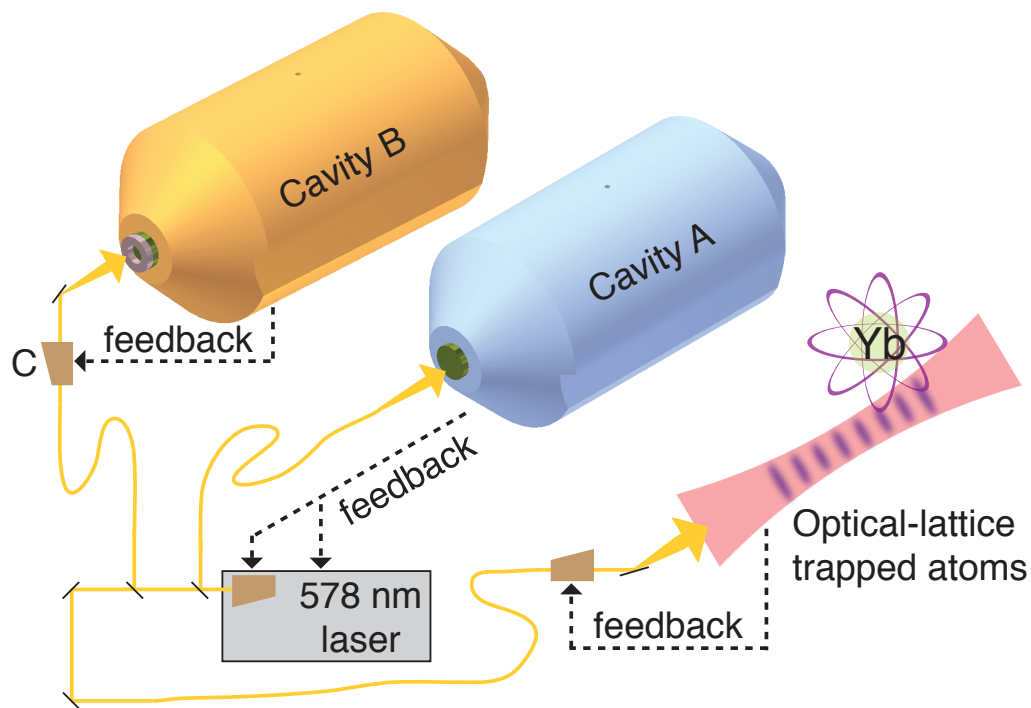


Figure 3.8: Setup for measuring cavity noise processes. Laser light at 578 nm is incident on two independent, isolated optical cavities. Each cavity is composed of a rigid ULE spacer with optically bonded fused-silica mirror substrates. Feedback for laser frequency control is usually applied to acousto-optic modulators (brown trapezoids). The stabilized light probes the narrow clock transition in an ultracold sample of ytterbium, confined in a one-dimensional optical lattice.

Viton hemispheres. By doing so, we were able to measure acceleration sensitivity (along gravity) as low as  $1 \times 10^{-11}/(\text{m/s}^2)$ . The vacuum chamber and optics coupling light to the cavity sat on vibration isolators (one cavity on an active system, the other passive). Each system was located in a different part of the laboratory in independent, closed, acoustic-shielded chambers. Optical links between the isolated systems and the laser source were made with optical fiber using active phase stabilization [169]. Free-space optical paths were generally in closed boxes to reduce air currents. The free-running 578 nm laser light was locked to Cavity A using PDH stabilization, with fast electronic feedback to an AOM that was common to all optical paths, and slow electronic feedback to a PZT on the laser source Fig. 3.8. Thus, light incident on both cavities was phase-stabilized to Cavity A.

To measure the laser frequency noise spectrum, an additional AOM was used to tune laser light incident on Cavity B into resonance, and the PDH signal of Cavity B served as a frequency discriminator. The frequency noise spectrum of one<sup>6</sup> cavity-stabilized laser is shown in the top panel of Fig. 3.9. The noise spectrum approaches the projected thermal noise for Fourier components around 1 Hz; at higher frequencies, the spectrum is approximately white, with several spikes attributed to seismic noise on one of the cavities.

To measure laser frequency stability, the PDH signal from Cavity B was filtered and fed to an AOM to lock the laser frequency of the second beam to the resonance of this cavity. This AOM frequency thus provided the difference between the two cavities, and was counted to determine the frequency stability. The stability shown in the middle panel of Fig. 3.9 used counting data from an Agilent 53132 (blue points) and a Stanford SR620 (black points), and measurements made using a Pendulum CNT-91 (not shown) gave similar measures of stability. During typical best performance, for averaging times below 10 s we observe an instability as low as  $2 \times 10^{-16}$ . Less ideal data sets give a measure closer to  $3 \times 10^{-16}$ . For averaging times longer than 10 s, laser instability typically increases due to nonlinear drifts of one or both cavities. We also measured the laser power spectrum, finding a linewidth of 250 mHz.

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<sup>6</sup> By “one” cavity we mean that we measured the noise between the two cavities, and divided the result by  $\sqrt{2}$ .

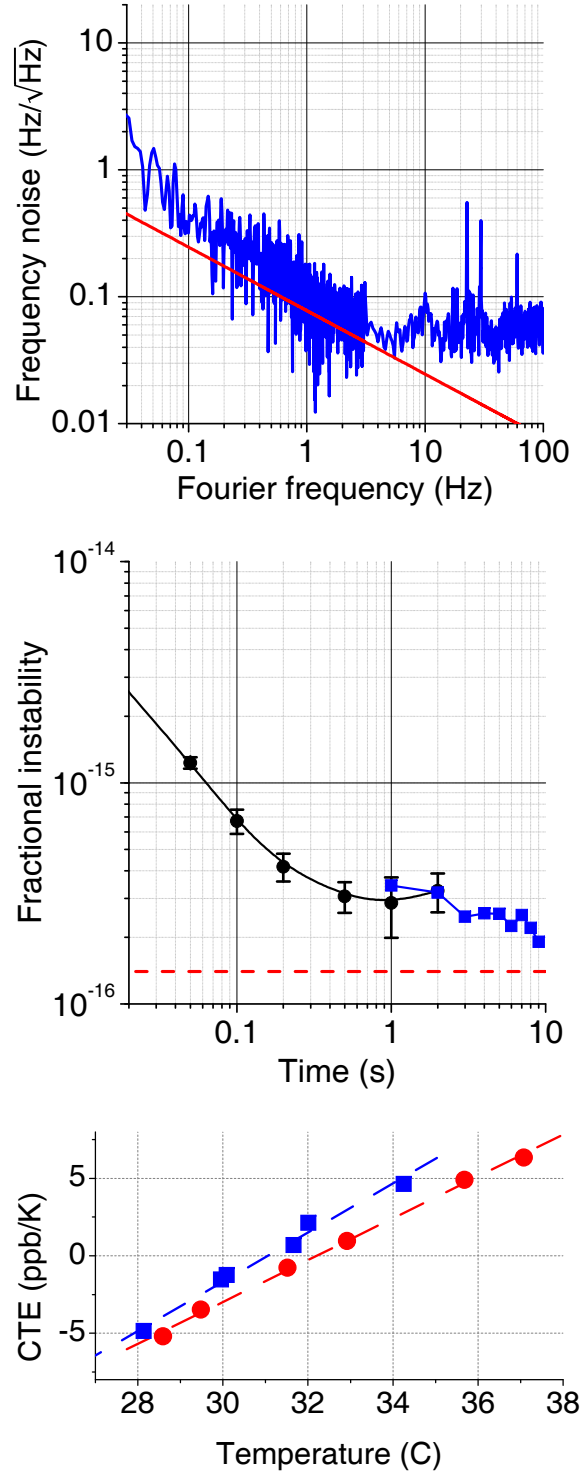


Figure 3.9: Top: Frequency noise spectrum (blue data) and theoretical estimate of the thermal noise (red line). Middle: Fractional frequency instability of one cavity. Blue squares derive from frequency counting with an Agilent 53132 counter [170] (1 s gate time, juxtaposed data set, with linear drift of 250 mHz/s removed), and black circles are from an SRS 620 counter (using a built-in Allan deviation tool, 1- $\sigma$  error bars shown). Bottom: Measurements of the coefficient of thermal expansion (CTE) for Cavity A (red circles) and Cavity B (blue squares), both of which cross zero just above 30°C.

Reaching this level of stability required careful attention to other noise sources beyond the thermal noise. As mentioned above, one well-known contributor is cavity length changes driven by acceleration-induced deformation. We measured this contribution by placing the cavities on a piezo-actuated “shaking” table, and we found both cavities had predominantly white noise spectra for Fourier components from 1–100 Hz, save for a few spikes near 20, 30, and 60 Hz.<sup>7</sup> For one cavity, the acceleration-induced frequency noise floor was very close to the observed frequency noise floor between the two cavities, roughly  $0.05 \text{ Hz}/\sqrt{\text{Hz}}$  at Fourier components above 1 Hz.

Other noise contributors include cavity length changes driven heating associated with absorption of the 578 nm light, uncompensated path noise fluctuations, and technical noise sources such as residual amplitude modulation (RAM) from the EOM, photon shot noise upon photodetection, stray etaloning effects, and electrical ground loops in the feedback system. We checked for noise associated with laser intensity fluctuations, and found the contribution to small:  $0.01 \text{ Hz}/\sqrt{\text{Hz}}$  at Fourier components of 1 Hz, and dropping for higher Fourier frequencies. We tested for path fluctuations (which could be caused by improper fiber noise cancellation or by fluctuations of the small free space paths before and after the fiber) and found their contribution to be 5–10 times smaller than the observed frequency noise in Fig. 3.9. We also measured the sensitivity to background gas inside the cavity, finding a “pressure shift” of  $25 \text{ Hz}/\mu\text{Torr}$ . With a base pressure of  $2.5 \mu\text{Torr}$ , this leads to a sizable shift of the cavity resonance; however, we expect the pressure to be reasonably constant on timescales up to 1 s. Finally, we measured the effects of technical noise sources (including shot noise) by analyzing the PDH signal when the light was tuned far away from the cavity resonance. This measurement revealed white noise floors of 0.01 and  $0.05 \text{ Hz}/\sqrt{\text{Hz}}$  for the two cavities, which, in the latter case, is roughly consistent with the observed frequency noise floor between the two cavities Fig. 3.9 for Fourier components above 1 Hz.

To minimize thermal drift of the cavities’ resonances, we engineered the coefficient of thermal expansion (CTE) to cross zero near room temperature. Because fused-silica mirrors have a much

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<sup>7</sup> These particular frequencies also dominated the acceleration spectrum of the lab floor, though we did find certain locations (near to the pillars that support the ceiling) that were better than others.

larger CTE (+500 ppb/K, with  $1 \text{ ppb} = 10^{-9}$ ) than the ULE spacer ( $\pm 30 \text{ ppb/K}$ ) to which they are contacted, temperature changes create stress, which bends the mirror substrate and introduces a larger CTE for the composite cavity ( $\text{CTE}_{\text{cav}}$ ) than for ULE alone. To compensate this effect and achieve a very small  $\text{CTE}_{\text{cav}}$ , we took advantage of the CTE dependence of ULE on  $\text{TiO}_2$  doping level and temperature [171]. By obtaining a ULE piece with doping levels corresponding to a room-temperature CTE of  $-40 \text{ ppb/K}$ , we were able to tune Cavity A temperature so that, combined with the mirror-bending effect, we observed a  $\text{CTE}_{\text{cav}}$  zero crossing at  $32.2(1)^\circ\text{C}$  (Fig. 3.9, bottom panel). At this temperature, which is conveniently just above room temperature,  $\text{CTE}_{\text{cav}} < 0.2 \text{ ppb/K}$ , minimizing thermal-driven drifts of the cavity. For Cavity B, we located a piece of ULE with small, negative CTE at room temperature and, following the procedure of [172], contacted ULE rings to the back side of the fused-silica mirrors. These rings largely prevent mirror bending from CTE mismatch with the spacer. We again observed a  $\text{CTE}_{\text{cav}}$  zero crossing, this time at  $31.1(1)^\circ\text{C}$ . After characterizing  $\text{CTE}_{\text{cav}}$  for each cavity, we installed radiative heat shields (low-emissivity, polished aluminium) between the temperature-stabilized vacuum chambers and each FP cavity. These shields reduce radiative heat transfer, which at first heats only the mirrors due to their small thermal mass.

### 3.6 Narrow atomic spectra and high clock stability

With the performance highlighted above, the cavity-stabilized laser serves well as a low-noise LO to probe the narrow clock transition of an optical-frequency standard. The first benefit of the low-noise LO is its ability to coherently excite the clock transition for long times (allowing a narrower linewidth). By probing the transition for 0.9 s and stepping the LO frequency by 0.25 Hz every experimental cycle, we resolved 1 Hz linewidth (FWHM) atomic spectra as in Fig. 3.10. With a transition frequency of 518 THz, this corresponds to a line quality factor of  $Q > 5 \times 10^{14}$ , the highest achieved for any form of coherent spectroscopy [173, 174]. Combined with a good measurement signal-to-noise ratio, this makes it possible to achieve very high clock stability.

Although the 0.9 s probe time enables very narrow atomic spectra, it leaves the atom lock



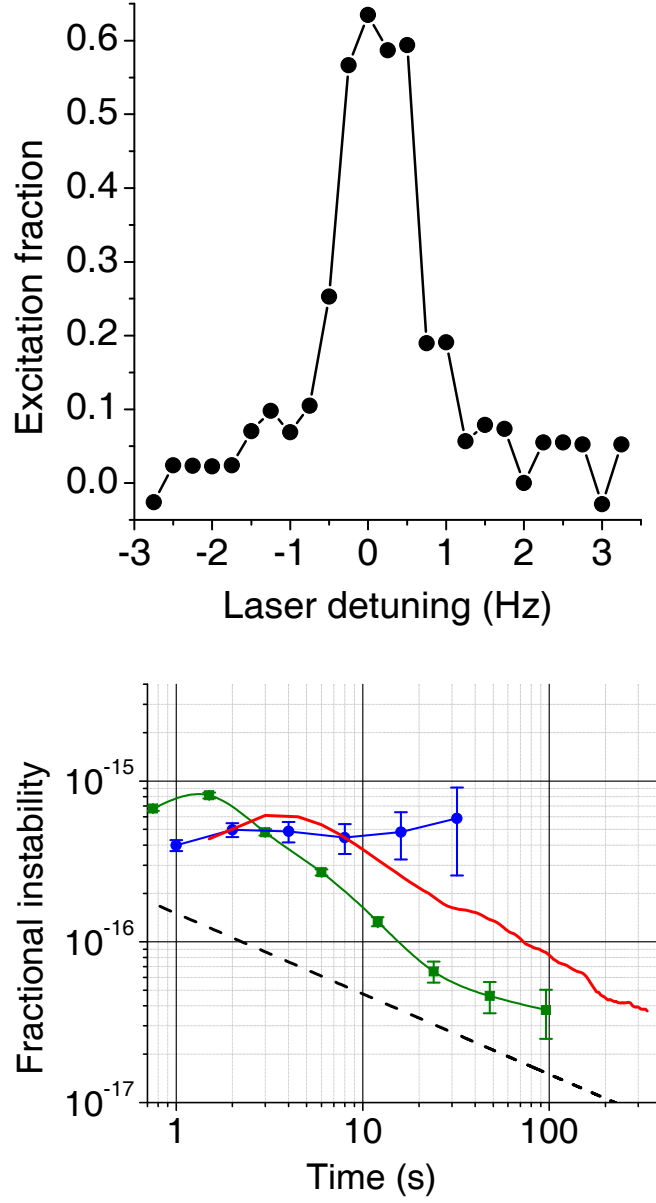


Figure 3.10: Top: Optical clock transition spectrum of neutral ytterbium atoms. The LO frequency is stepped by 0.25 Hz every cycle, with a probe time of 0.9 s, resolving a spectral linewidth of 1 Hz, FWHM (no averaging). Bottom: Instability evaluation of the ytterbium clock using the atomic transition. Blue circles use the atomic excitation as an (out-of-loop) frequency discriminator for measuring the LO frequency. Green squares give the in-loop stability (from the error signal) when the LO is locked to the atomic transition. The Dick-effect-limited instability (black dashed line) is  $1.5 \times 10^{-16}/\sqrt{\tau}$ . The red curve indicates the stability for interleaved measurements used to assess systematic shifts. The error bars are  $1-\sigma$ .

sensitive to short-time laser frequency excursions, which occasionally exceed the  $\sim 1$  Hz capture range of the lock. For this reason, we chose to operate the system with a 0.3 s probe time ( $\Delta\nu \approx 3$  Hz), 40 % of the 0.75 s total cycle. Under these conditions, and with the LO frequency noise spectrum from Fig. 3.9, we calculated the Dick limit to be  $1.5 \times 10^{-16}/\sqrt{\tau}$ , (dashed line in lower panel of Fig. 3.10), an order of magnitude of improvement over our previous LO [165].

To rigorously assess clock instability (consisting of the LO stabilized to the ytterbium transition), it must be compared to another standard with even lower instability. Anticipating previously unobserved stability levels with this individual system, we instead evaluated the noise levels that determined the clock instability. We tuned the LO frequency on-resonance with the atomic transition and used the measured excitation as a frequency discriminator. This out-of-loop measurement is sensitive not only to LO frequency instability, but also to the noise terms that set the mid-to-long-term instability of the optical standard (including the Dick effect and detection noise of the atom system). The results of this measurement are shown as blue circles in the lower panel of Fig. 3.10), indicating that the optical clock system supports an instability of  $\lesssim 5 \times 10^{-16}$  after just one measurement cycle.

Rather than just scanning across or sitting on the side of the atomic line, we can instead close the loop and lock the LO to the atomic transition. This is accomplished via slow feedback to the pre-cavity AOM from a digital synthesizer that is controlled by the microprocessor (Fig. 3.7). The correction signals are found by digitally integrating an error signal that is derived from repeated excitation measurements on each side of the atomic transition. With proper feedback, the instability can begin averaging down, as suggested by the green squares in Fig. 3.10. This is the in-loop error signal stability of the LO lock to the atomic transition, and gives a lower limit to the expected clock instability. At 1 s, we see that our aggressive choice of feedback gain degrades the LO stability. However, by 2 s we begin averaging down, faster than  $1/\sqrt{\tau}$ , so that after 20 s of closed-loop operation, we can reach the anticipated  $5 \times 10^{-16}/\sqrt{\tau}$  indicated by the out-of-loop signal. Construction of a second ytterbium optical lattice clock, currently under way, will enable even more direct measure of the improved stability.

It's also interesting to calculate what the Dick effect instability would be for several different configurations. For the same parameters, but with Ramsey spectroscopy, the Dick limit is  $1.2 \times 10^{-16}$ , a modest improvement. With a shorter cycle time, the Dick effect is sensitive at somewhat higher Fourier components, where the noise spectrum is lower. For example, with a cycle time of 350 ms and Ramsey interrogation time of 150 ms (130 ms dark time and 10 ms pulses), the Dick limit is  $1.0 \times 10^{-16}$ . This latter configuration was used during measurements of the collision shift cancelation (Sec. 5.6).

In addition to the Dick effect, the noise processes that presently affect the ytterbium clock instability (at  $\tau =$  one cycle) include atom detection noise, measured at  $\sim 1 \times 10^{-16}$  (equivalent to a S/N of 50), and uncompensated optical path phase noise on the ytterbium apparatus measured at  $\leq 2 \times 10^{-16}$ . Here, we emphasize a key point: by sufficiently reducing the Dick effect, we have more fully enabled the benefits afforded by the signal-to-noise ratio of a large atom ensemble to achieve this unprecedented level of stability.

This stability enables high-precision frequency measurements at faster speeds than ever before, including characterization of systematic shifts of the ytterbium clock transition. Several important systematic shifts can be studied by interleaving the clock operation between two conditions and looking for a frequency shift. Typically, the parameter of interest (e.g. the atomic density or the lattice power) is toggled every 2 clock cycles between two different values. The microprocessor has a separate set of integrators for each case, and the difference between the correction signals applied to the AOM reveals the shift. Importantly, this method is largely insensitive to laser drift because it subtracts out in the difference of the correction signals.

The red trace in Fig. 3.10 shows the stability of such a measurement, enabling precision at  $< 8 \times 10^{-17}$  at 100 s and averaging down as  $1/\sqrt{\tau}$ . Note that this observed instability is consistent with  $5 \times 10^{-16}/\sqrt{\tau}$  for normal single operation, accounting for the quadrature sum of uncorrelated noise between the two-setting-interleaved clock operation, as well as the extra cycle time required for dual operation.

Still, lattice clocks offer yet more untapped potential in terms of their stability. The Dick

limit must be lowered by yet another order of magnitude to reach possible quantum projection noise limits. Efforts to reduce the preparation time in the experimental cycle will help significantly [175, 176]. The effect will continue to get smaller as the LO is further improved, including further reduction of the cavity thermal noise. Many worthwhile efforts can be made here, focusing on one or more of the critical cavity parameters described above, such as increasing the beam size on the mirror (either with larger ROC mirrors, or with higher-order cavity excitation [166]) or cryogenic cavity cooling [160, 177]. Yet longer cavities may be difficult; but, to make the cavity effectively longer, a multiple-mirror cavity could be used [46].

Recently, there has also been renewed interest in using quantum absorbers for a high stability (but not necessarily high accuracy) reference. Some of these ideas include spectral hole burning in cryogenically-cooled crystals [178, 179], collective emission of ultracold atoms [180, 181], and spectroscopy of narrow transitions in atoms in a cavity [182] or even atoms in a thermal beam. As these techniques (as well as traditional cavity-stabilization) progress, it will be exciting to use the resulting stable sources to probe extremely narrow transitions in the lattice clocks, thereby reaching yet higher levels of clock stability.

## Chapter 4

### Lattice Light Shifts

As discussed in Ch. 2, the Stark shift produced by an intense laser field tightly confines the atoms to a spatial extent smaller than the wavelength of light. The interaction between the trapping light and the atom is dominated by a scalar light shift that, near the magic wavelength, is carefully balanced for the ground and excited clock states. Thus, the *net* scalar Stark shift to the clock transition is nearly zero, and higher-order terms become relevant. We can write the total light shift as

$$\Delta\nu_L = \alpha(\omega_L) I + \beta(\omega_L) I^2 + (n + \tfrac{1}{2}) \gamma(\omega_L) \sqrt{I} \quad (4.1)$$

with  $\omega_L$  the frequency of the confining lattice light,  $I$  the lattice light intensity, and  $n$  the motional quantum number of the confined atom. With  $\omega_L$  chosen to minimize  $\alpha$ , the higher-order coefficients ( $\beta$  and  $\gamma$ ) are likely to be non-zero. In this chapter, we will first examine the measurements used to identify the magic wavelength. Next, we will examine the higher-order terms ( $\beta$  and  $\gamma$ ). Finally, we will consider the vector light shift, which causes a differential shift between the magnetic substates  $m_F$ .

#### 4.1 Experimental determination of the magic wavelength

In 2007, the magic wavelength for  $^{174}\text{Yb}$  was found with an uncertainty of 35 MHz by thoroughly studying the dependence of the clock frequency on lattice intensity [126, 92]. The shift was found to be mostly linear in  $I$  and linear in detuning away from the magic wavelength. To

find the magic wavelength for  $^{171}\text{Yb}$  required only a minimal effort to evaluate the small change of the magic wavelength due to the isotope shifts and hyperfine splittings of the nearby  $^3S_1$  and  $^3D_1$  states. However, because  $^{171}\text{Yb}$  offered a potentially lower total clock uncertainty, we also desired to make a better measurement, which required some care to avoid errors from hyperpolarizability and collision shifts. The hyperpolarizability was also previously measured by scanning over nearby two-photon resonances (see [126] and below), while the collision shift coefficient was calibrated for a particular atom number (see Ch. 5), and the change in density induced by a change in lattice depth  $U$  was taken to be  $U^{3/4}$  (see Appendix A.1).

The blue points of Fig. 4.1 show the first measurement of the magic frequency in  $^{171}\text{Yb}$ , which were made in 2008 [43]. The frequency shift induced by a change in the lattice power was measured relative to the Ca optical clock, with a frequency comb used to span the large frequency gap (Sec. 7.1). Because the comb was being operated as part of the measurement, it was also convenient to lock the lattice laser frequency the comb by monitoring the beat signal between one comb tooth and the lattice laser, with slow feedback to an intra-cavity PZT (Sec. 3.2). Rather than spread the experimental effort over many laser detunings and intensities, we concentrated on just two intensity levels and five detunings. The shift shown in the figure is the difference in clock frequency for the two intensities, extrapolated to full intensity ( $I \simeq 130 \text{ kW/cm}^2$ , or  $\sim 450 E_r$ ) and corrected for the associated hyperpolarizability and collision shifts, for each detuning.

The final error bar associated with the linear Stark shift can be assigned in two ways. First, one could fit a line to the data (shown in solid blue), weighted by the individual error bars, and use the goodness of fit to determine the uncertainty in the x-intercept. Second, one could take the single measurement nearest the zero-crossing as the clock operation point, and take that single measurement's error bar as the clock's uncertainty. For these data, it turned out that the latter gave a smaller error bar; both determinations are shown in the lower panel of the figure (blue points). We reported the magic frequency as  $394\,798\,329(10) \text{ MHz}$ , which corresponds to an isotope shift  $\nu_{magic}^{174} - \nu_{magic}^{171} = 1146(36) \text{ MHz}$ . The clock uncertainty from the linear Stark effect is  $1.7 \times 10^{-16}$ .

A second measurement of the magic frequency was performed in 2010 under some very

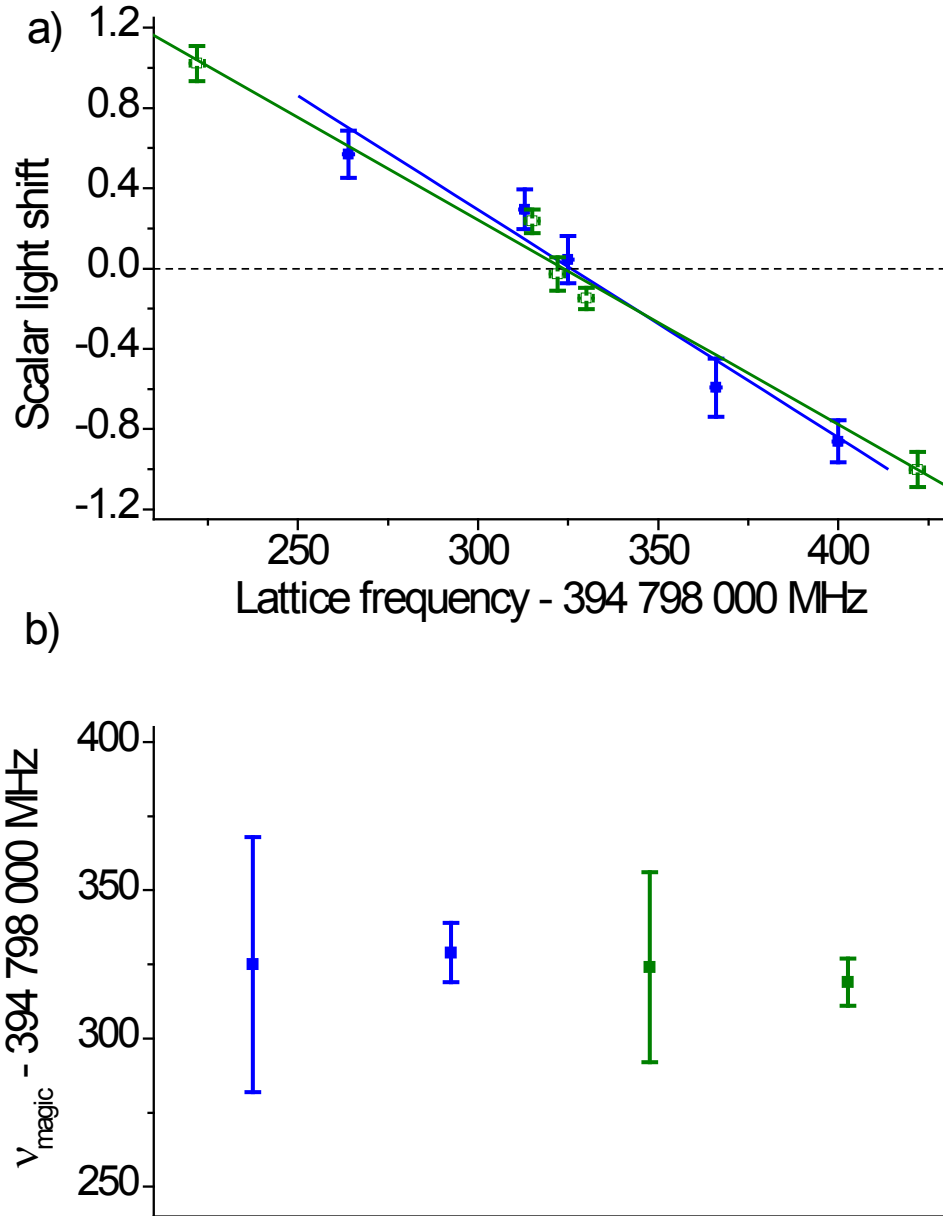


Figure 4.1: a) Stark shift vs. lattice frequency. The blue points were measured with Rabi spectroscopy relative to the Ca clock, while the green points were measured with Ramsey spectroscopy relative to the stable optical cavity. b) Several determinations of the magic frequency are found to agree well. The magic frequency can be found with a weighted least squares fit, or by simply taking the best measurement near the zero-crossing. For both the blue and green measurements (which correspond to the data sets in part a) of this figure), the latter case gave the smaller error bar.

different clock operations. We switched to a Ramsey sequence instead of Rabi, which provided the means for canceling the collision shift. With the collision shift mostly canceled, any change in collision shift associated with changing the lattice depth was very small (as was the corresponding uncertainty). Another improvement was to measure the shift relative to the optical cavity rather than the Ca clock (see Sec. 3.6.) By interleaving the two lattice depths and finding the shift between them, we placed a yet tighter constraint on the magic frequency, as shown in the green points in Fig. 4.1. Because the frequency comb was not used for the measurement, we instead referenced the laser frequency to a small ULE cavity, and made occasional (once per day) short calibrations with the frequency comb to ensure the cavity had not drifted a significant amount. The lower panel of the figure again shows the two determinations of the magic frequency (green points). The second determination of the magic frequency yielded 394 798 319(8) MHz, which agrees well with the first measurement.

Future measurements will benefit from several recent improvements. First, we have shown the collision shift can be canceled at a very small level (Sec. 5.6), which should prevent any spurious collisional effects from contaminating the measurement. Second, recent improvements to the clock stability should allow for smaller statistical error bars. Finally, a resonant build-up cavity around the atoms should substantially increase the lattice intensity, providing the leverage to make small effects large enough to see. With hopes of constraining the first-order light shift to  $10^{-17}$  or smaller, it will be necessary to (re-)visit other higher-order light shifts, described below.

## 4.2 Hyperpolarizability: second-order Stark shifts

Having studied the linear term in Eq. 4.1, we now turn our attention to effects which are quadratic in intensity (quartic in electric field). Termed hyperpolarizability, these effects are expected to be quite small, unless the magic wavelength is near any two-photon transitions from the excited clock state to a higher-lying state [40, 41, 125]. For Sr, the nearest of these resonances is 5 nm away from the magic wavelength, and hyperpolarizability effects are shown to be quite small [183]. With Yb, however, it seems luck was not on our side. The nearest resonance is detuned by



only 183 GHz from the magic frequency. There are two other nearby resonances, though these are detuned by a few nanometers.

We measured the effects of these resonances by tuning the lattice very near the resonance and monitoring the clock transition. Near the resonance, the clock spectrum became highly shifted and broadened. Fitting the measured shifts as a function of detuning allowed for a measure of the line strength, and subsequent extrapolation back to the magic wavelength determined that the effects on normal clock operation are small, but non-negligible. The results were published in [126] and in a previous thesis [92] and are not re-printed here. Table 4.1 lists the resonances, their detunings, and the associated shifts.

The frequency shifts listed in the table are those measured with a linearly polarized lattice. With circular polarization, the  $^3P_0 \rightarrow ^3P_0$  resonance is forbidden [126]. This fact, together with the opposite sign of shift associated with the  $^3P_0 \rightarrow ^3P_2$  transition, means there exists a “magic” polarization that fully cancels the hyperpolarizability effect [185]. This idea is depicted in Fig. 4.2. Using the measured shift coefficients and the predicted polarization dependence [185], the green curve shows the total hyperpolarizability dependence on polarization (plotted versus the ellipticity angle, where  $\pi/4$  corresponds to circular polarization). The curve crosses through zero at “magic ellipticity” of  $0.68(7) \times \frac{\pi}{4}$ .

Efforts to better locate the magic wavelength will likely be hindered somewhat by the non-zero hyperpolarizability shift. Measuring the frequency dependence at multiple intensities (includ-

Table 4.1: List of the two-photon resonances from  $6s6p\ ^3P_0$  that contribute to the hyperpolarizability in Yb. The detuning from the magic frequency is given, along with the predicted shift at the magic wavelength for a linearly polarized 1D lattice (500 recoil depth), as determined in [126]. Note that the  $^3P_0 \rightarrow ^3P_1$  transition is forbidden by two-photon selection rules [184].

| State         | Detuning (THz)    | Shift (Hz) @ 500 $E_r$ |
|---------------|-------------------|------------------------|
| $6s8p\ ^3P_0$ | $2 \times -0.183$ | 0.20(3)                |
| $6s8p\ ^3P_1$ | $2 \times 0.984$  | —                      |
| $6s8p\ ^3P_2$ | $2 \times 2.7$    | -.038(8)               |
| $6s5f\ ^3F_2$ | $2 \times -2.9$   | .004(10)               |

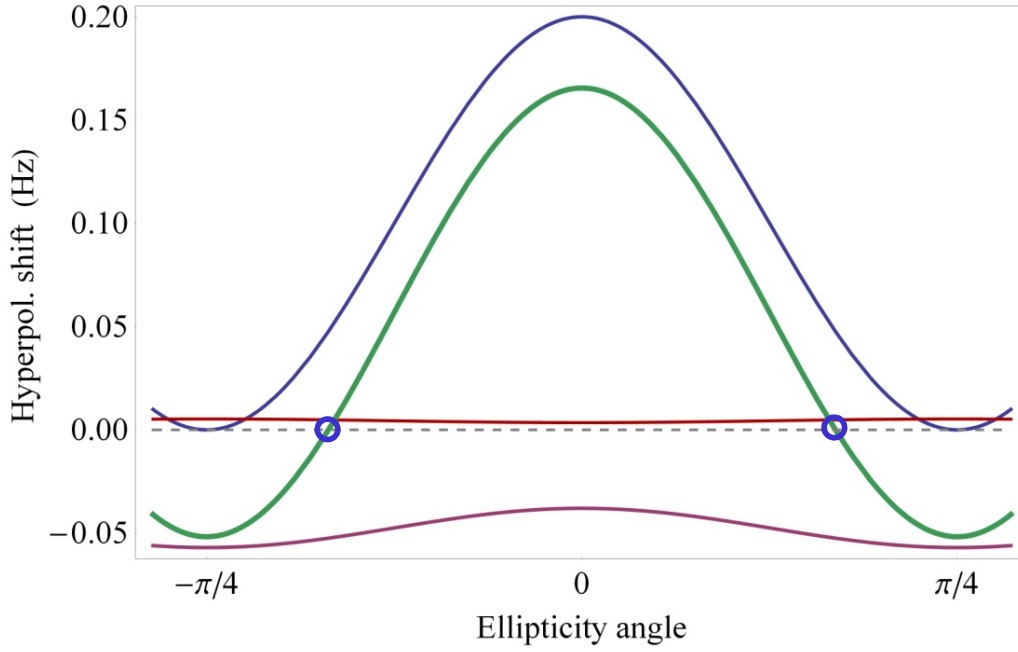


Figure 4.2: Predicted polarization dependence of the hyperpolarizability shift. The blue, purple, and red curves correspond to the shifts associated with the  ${}^3P_0$ ,  ${}^3P_2$ , and  ${}^3F_2$  resonances, respectively, for a  $500 E_r$  lattice depth. The x-axis is the ellipticity, given as the ratio of the ellipse’s major and minor axes, with 0 corresponding to linear polarization and  $\pi/4$  to circular polarization. The green curve gives the sum of the three resonances, and crosses through zero at a “magic ellipticity” of  $0.68(7) \times \pi/4$ .

ing very large intensities) should allow for simultaneous constraints on the linear and quadratic pieces. Fortunately, the quadratic scaling means that the hyperpolarizability shift can be quite small in weaker traps. Even without further measurement, the clock uncertainty associated with hyperpolarizability in a 200  $E_r$  lattice is  $1 \times 10^{-17}$ .

### 4.3 Multi-polar polarizability

Early theoretical work proposing Sr and Yb as lattice clock candidates also considered magnetic dipole transitions (i.e.  $J = 0 \rightarrow J = 1$ ) and electric quadrupole transitions (i.e.  $J = 0 \rightarrow J = 2$ ) in addition to electric dipole [40, 41]. The initial thinking was that, because the related clock shift also scales linearly with intensity, these contributions would only cause a negligible shift to the magic wavelength, with the relevant polarizabilities ( $\alpha$ ) scaling as  $\alpha_{M1} \simeq \alpha_{E2} \lesssim 10^{-6} \alpha_{E1}$ . However, subsequent theoretical work pointed out that in a standing wave, the spatial distribution of the magnetic field is out of phase with the electric field. As such, the total potential can be written [127]

$$U(z) = U_{E1} \cos^2[kz] + (U_{M1} + U_{E2}) \sin^2[kz]. \quad (4.2)$$

For a 1D lattice, the frequency shift associated with these higher-pole terms is

$$\Delta\nu_{(M1,E2)} = (n + 1/2) \gamma \sqrt{I} \quad (4.3)$$

with  $I$  the lattice intensity,  $n$  the motional quantum number for the lattice-trapped atom, and  $\gamma$  a parameter that is related to the atomic polarizability. For typical operating conditions,  $\Delta\nu_{(M1,E2)}$  could be as large as  $10^{-16}$  fractionally. Even if the effect were that large, it would be difficult to resolve the shift associated with the different motional states  $n$ , which means instead that the average value ( $\langle n \rangle \approx 2.5$  for Yb) should be taken. In higher-dimensional lattices, the effect could be more pronounced, since the spatial distribution is not as simple as Eq. 4.2 suggests [127], although there may be certain configurations that minimize the effect [186].

Recent experimental work with Sr did not resolve this effect at the level of  $10^{-17}$ , while no careful measurement of the effect has been performed with Yb. The same future measurements to

further refine the scalar and hyperpolarizability terms will also need to consider this multi-polar effect, although the weaker intensity scaling ( $I^{1/2}$ ) means it is harder to see.

## 4.4 Vector Stark shift

### 4.4.1 Vector shift in 1D lattice

The vector Stark shift (Eq. 2.29) is an  $m_F$ -odd shift which is non-zero in the presence of elliptically polarized light. For lattice clock systems like Sr and Yb, the vector polarizability of the ground state is much smaller than the excited state, so we will ignore it. Because of the  $m_F$  scaling, the vector shift is often thought of as an effective magnetic field along the direction of propagation *veck*. In the presence of a static magnetic field  $\vec{B}$ , the vector sum of the two “magnetic” fields determines the total Zeeman-like splitting. For the special case of  $\vec{B} \perp \vec{k}$ , a quadrature sum determines the combined Zeeman-like dependence [187, 135]:

$$\Delta\nu_{m_F} = m_F \sqrt{([g_I + g_{\text{HFS}}] \mu_B B)^2 + \left(\frac{1}{4} \alpha_{\text{vs}} A \mathcal{E}^2\right)^2}. \quad (4.4)$$

Subtracting the Zeeman-shift of the ground state determines the total Zeeman-like sensitivity of the transition. With linear polarization, the vector light shift is almost certainly smaller than the Zeeman shift; for that reason, choosing  $\vec{B}$  orthogonal to  $\vec{k}$  only further reduces the observed vector shift.

In Fig. 4.3, we measure the vector shift in a 1D lattice by introducing ellipticity into the lattice field. Shown is the vector shift inferred from the splitting of the  $\pi$  transitions as a function of the quarter waveplate angle. Data of different color corresponds to different magnetic field values, which was oriented orthogonal to the lattice, and the mutual agreement confirms that we have correctly included the combined effects of Zeeman and vector shifts.

For typical clock operation, the vector shift is expected to be small for several reasons. First, the polarization is primarily linear; even with vacuum viewport birefringence, the ellipticity is  $A \lesssim 0.1$ . Second, because we orient the magnetic field perpendicular to the lattice, the quadrature sum described above further suppresses the shift. For  $B \simeq 1$  G and  $A = 0.1$ , the residual shift is

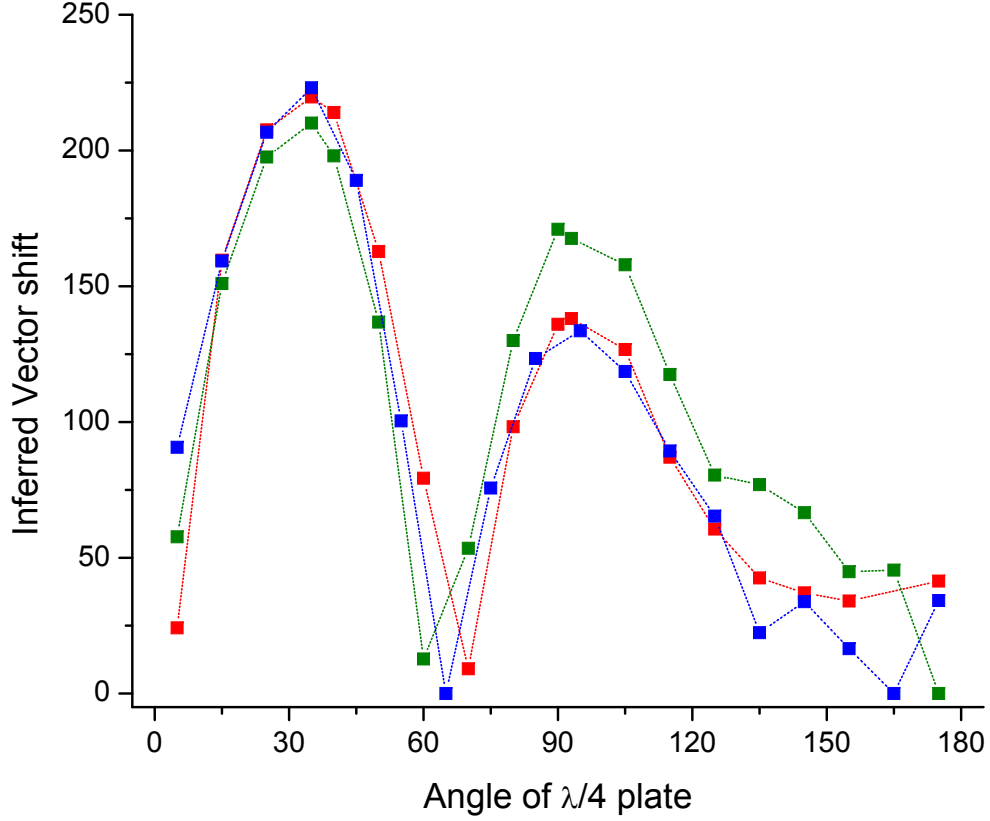


Figure 4.3: Measurements of the vector Stark shift in a 1D lattice with a crossed magnetic field. The vector shift was made non-zero by introducing ellipticity to the lattice via a quarter waveplate. The blue points were acquired with a 1.1 G magnetic field (1 Gauss =  $10^{-4}$  Tesla); green points with a 0.55 G field; and red points with no applied field (and residual field less than 30 mG). The magnetic field was oriented orthogonal to the lattice. The agreement between the three curves verifies our analysis of the combined Zeeman and vector Stark effects as they affect the splitting of the  $\pi$  transitions. The lattice intensity for these data was approximately  $125 \text{ kW/cm}^2$ , or about  $450 E_r$ .

$\Delta\nu_{\text{vs}} \sim \pm 0.4$  Hz. Finally, averaging over both  $\pi$  transitions should fully cancel any residual shift.

#### 4.4.2 Possibility for uncanceled vector shifts

This cancelation assumes there is no other physics that would shift the average of the two  $m_F$  states. However, this was recently called into question [188]. We looked for a shift of the center by alternating between linear and circular polarization at several magnetic field values and checking for a clock shift. It was necessary to correct the data for changes in the hyperpolarizability and second-order Zeeman shifts. The results are shown in Fig. 4.4; no clear trend was observed.

#### 4.4.3 Vector shift in a 2D lattice

As mentioned in Sec. 2.3.3, we configured our 2D lattice with two independent beams (rather than one folded beam) for maximal experimental flexibility, and with crossed polarization (rather than matched) so that the intensity distribution did not depend on the time-phase between the two standing waves. However, below we will show that the local polarization vector (and hence the vector Stark shift) does care about the time-phase, and allowing that phase to freely drift could have negative effects on the precision spectroscopy we aim to achieve.

Consider the geometry in Fig. 4.5. Two beams, one traveling along  $\hat{x}$  and one along  $\hat{y}$ , intersect the atomic cloud, with a relative phase between them  $\theta = k_x d_1 + k_y d_3$ . Each beam is retro-reflected and passes through the atomic cloud a second time, with additional phases  $\phi_x = k_x d_2$  and  $\phi_y = k_y d_4$ , to produce standing waves along  $\hat{x}$  and  $\hat{y}$ . The standing wave along  $\hat{x}$  is linearly polarized along  $\hat{y}$ , and the standing wave along  $\hat{y}$  is linearly polarized along  $\hat{z}$ . While other crossed polarization geometries could be suitable, the motivation behind this particular geometry will be made clear later.

The total electric field  $E_T$  is given by the sum of the four traveling waves:

$$\begin{aligned} \vec{E}_T = & \left( E_1 e^{i(\omega_x t + k_x x)} + E_2 e^{i(\omega_x t - k_x x + 2\phi_x)} \right) \hat{y} \\ & + \left( E_3 e^{i(\omega_y t + k_y y + \theta)} + E_4 e^{i(\omega_y t - k_y y + \theta + 2\phi_y)} \right) \hat{z}. \end{aligned} \quad (4.5)$$

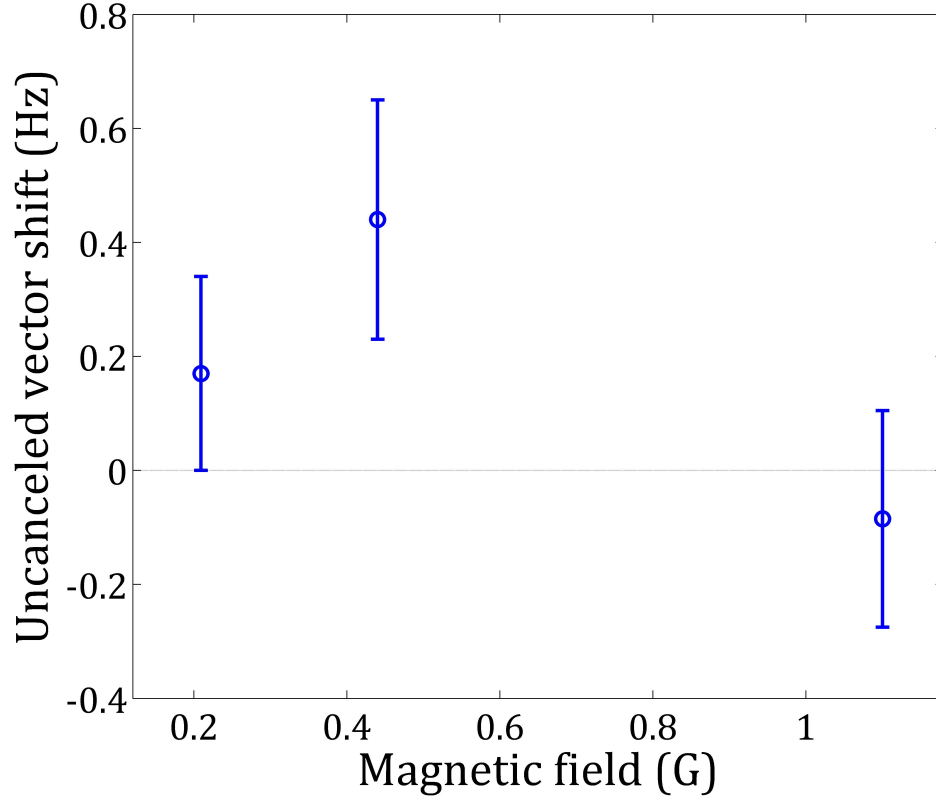


Figure 4.4: Measurement of the clock’s sensitivity to vector shift with circular polarization. This quantity was expected to be zero because we average over both  $\pi$  transitions, for which the dependence is opposite; however, Ref. [188] predicts otherwise. The y-axis shows the shift between circular polarization (where the effect is maximal) and linear polarization (where it is minimal). The data were acquired for several magnetic field values; no clear trend was observed.

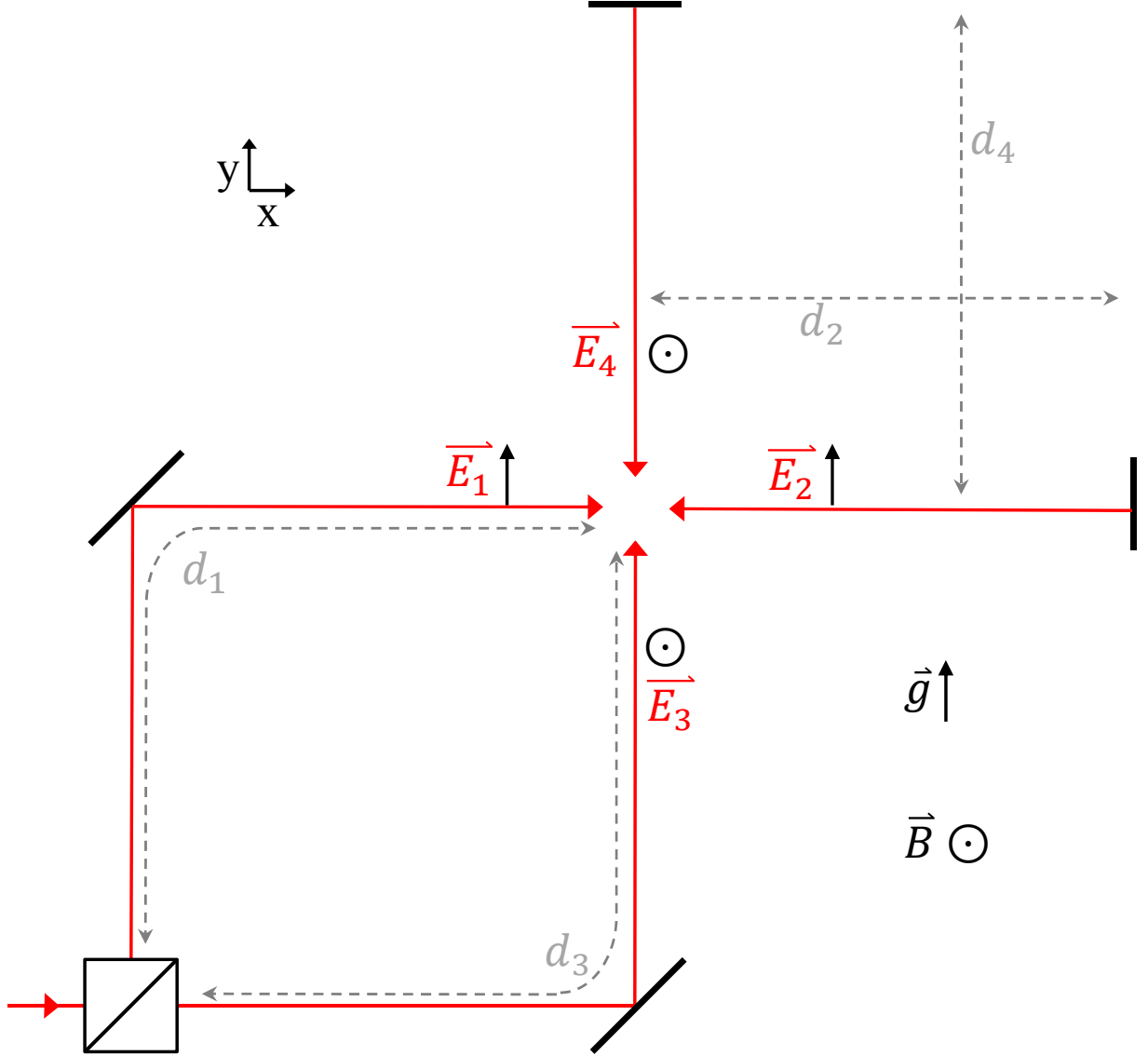


Figure 4.5: Shown is a diagram of the four beams that form the 2D lattice, including polarization vectors relative to the magnetic field direction and gravity. The relative phase between the forward beams (see main text) is  $\theta = k_x d_1 + k_y d_3$ , and the additional phase gained upon retroreflection is  $\phi_x = k_x d_2$  for the  $\hat{x}$ -lattice and  $\phi_y = k_y d_4$  for the  $\hat{y}$ -lattice.



The intensity distribution is proportional to the square of the electric field. For the simple case of equal power in each beam ( $E_0 = E_4 = E_3 = E_2 = E_1$ ), we have

$$\begin{aligned}\langle |E_T|^2 \rangle &= \frac{1}{2} E_T \cdot E_T^* \\ &= 2|E_0|^2 (\cos^2[k_x x - \phi_x] + \cos^2[k_y y - \phi_y])\end{aligned}\tag{4.6}$$

where the  $*$  denotes complex conjugation. We immediately see that the phases  $\phi_x$  and  $\phi_y$  cause only translations along the respective directions, while the relative phase term  $\theta$  has no effect on the intensity distribution, in agreement with Eq. 2.21.

The vector shift depends on the ellipticity of the field distribution, which can be calculated as a cross-product:

$$\begin{aligned}\Delta\nu_{\text{vs}} &= \frac{1}{4} \frac{m_F}{2F} i \alpha \vec{E}_T \times \vec{E}_T^* \\ &= -2 m_F \alpha |E_0|^2 \cos[k_x x - \phi_x] \cos[k_y y - \phi_y] \underbrace{\sin[\theta - \phi_x + \phi_y]}_{\phi_T} \hat{x}.\end{aligned}\tag{4.7}$$

The brace defines a new composite phase  $\phi_T$  which is the sum of all three phase terms; we will refer to this as the “time-phase.” For  $\phi_T = 0$ , the standing waves are in time-phase, and the polarization is always linear everywhere. For any other case, the standing waves are not in time-phase, and the field has some ellipticity. In our experiment,  $\phi_T$  is neither measured nor controlled, so the vector shift is generally non-zero. Moreover, any path-length fluctuations (caused by air currents or mirror vibrations, for example) will write noise onto  $\phi_T$  and onto the polarization of the 2D lattice.

As mentioned above, a non-zero  $\Delta\nu_{\text{vs}}$  is not a big hindrance, because it can be averaged away like the linear Zeeman shift; however, any non-negligible *line broadening* due to the vector shift is a hindrance. There are several reasons we might expect line broadening here. First, the intensity distribution in the 2D lattice is non-uniform, being highest in the center of the Gaussian beams but falling off quite quickly away from center. Second, fluctuations in  $\phi_T$  will cause the vector shift to vary throughout the spectroscopic interrogation. Finally, the case above (Eq. 4.7) assumed equal intensities in each beam; if this condition is not met, the polarization becomes spatially-dependent [116]. With these broadening mechanisms, a reasonable guess is that the vector shift broadening could be as large as half the maximum shift, or a few hundred hertz.

Fortunately, a simple trick can be used to clean up the polarization. By placing a small frequency offset between the two beams ( $\omega_3 \rightarrow \omega - \Delta\omega$  and  $\omega_1 \rightarrow \omega + \Delta\omega$ ), we can spin the polarization vector quickly – much faster than any of the decoherence mechanisms listed above – and wash out the effect. This is made apparent by considering the vector shift with this frequency modulation:

$$\Delta\nu_{\text{vs}} = 2 m_F \alpha |E_0|^2 \cos \left[ x \left( k - \frac{\Delta\omega}{c} \right) - \phi_x \right] \cos \left[ y \left( k + \frac{\Delta\omega}{c} \right) - \phi_y \right] \sin [2 t \Delta\omega - \phi_T] \hat{x} \quad (4.8)$$

where the relation  $\omega = c k$  has been used so as to include the corresponding change to the lattice spacing. Experimentally, we used a value of  $\Delta\omega/2\pi = 1$  MHz, for which the change in lattice spacing is only a few parts per billion. This value of  $\Delta\omega$  is significantly larger than the lattice trap frequencies, hence there should not be any additional heating or trap loss, but smaller than the uncertainty in the magic frequency, so that the Stark shift associated with tuning away from the the Stark-canceling condition is minimal.

The effect of the modulated polarization on clock spectroscopy is very similar to the way atomic motion affects clock spectroscopy – as a resolved sideband. Just as the atom's periodic motion in the lattice well produces a modulated spectrum with an unshifted carrier, the rapidly precessing polarization vector moves the effects of the vector Stark shift out to high frequency sidebands. The sidebands will be resolved if the modulation rate ( $\Delta\omega$ ) exceeds the fluctuations in the time-phase ( $\dot{\phi}_T$ ), which is easily satisfied for the large  $\Delta\omega$  chosen here. Experimentally, we observed the sidebands on the clock spectrum for  $\Delta\omega \approx 1$  kHz, but for larger values the modulation index became too small to efficiently excite the transition.

Eq. 4.8 treats the case of perfectly balanced beam intensities. In practice, this condition is never met due to losses in the beam path (e.g. reflections from vacuum viewports, retroreflector losses, etc), and the effect of imbalanced intensity is to create spatial-dependence in the polarization vector. Fortunately, the frequency offset technique is still effective at suppressing the vector shift even with intensity imbalance.

There is, however, one other source of vector shift for which the frequency offset does not

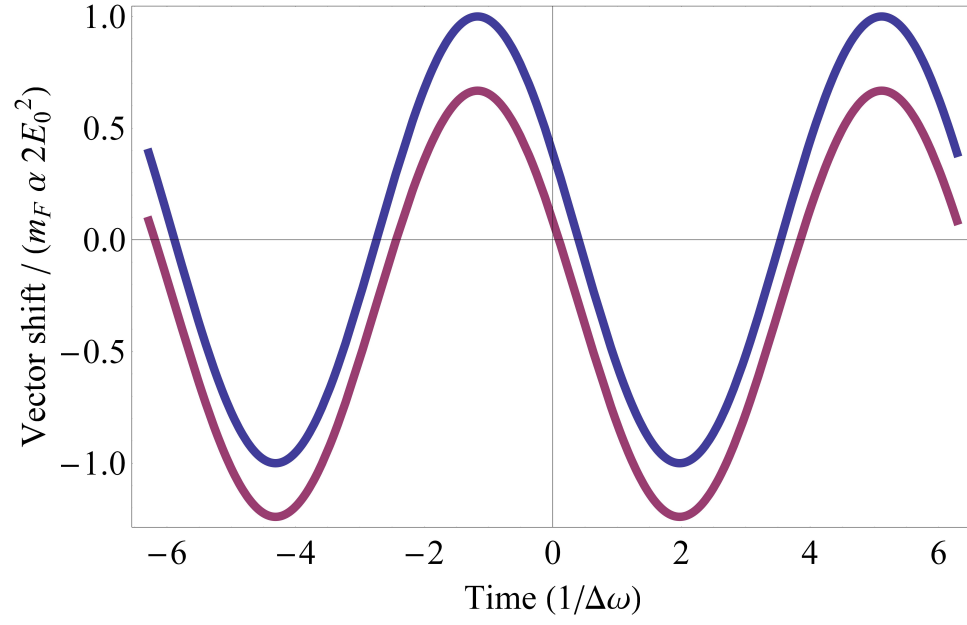


Figure 4.6: A frequency offset in a 2D lattice modulates the polarization and suppresses the vector shift. This is shown in the blue curve, for which the vector shift averages to zero. However, the purple curve highlights the fact that an intrinsic ellipticity in one or both of the lattice beams prevents perfect averaging.

help – any intrinsic ellipticity in the beams. That is, if the individual beams are not perfectly linear polarized, the additional ellipticity can cause vector shifts which do not completely average to zero, and hence which have a component at d.c. that affects the carrier. Fig. 4.6 demonstrates this by showing the polarization getting wrapped as predicted (blue curve) for perfect linear polarization; the purple curve, however, shows the time-dependent vector shift for the case of an ellipticity angle of 0.1. The time-dependence is present, but the curve does not average to zero.

In practice, it's quite difficult to make clean polarization. The best way would be to place high-quality optical polarizers inside the vacuum chamber; but since we have not done so, we are forced to accept any optical rotation caused by the vacuum windows' unwanted birefringence. Fortunately, in a 2D lattice we still have one more degree of freedom – the direction of the magnetic field. Going back to Eq. 4.5, we can now explain the choice of geometry. With  $\hat{x}$  and  $\hat{y}$  the two directions of strong confinement, we choose the  $B$ -field along  $\hat{z}$ , so that the intrinsic ellipticity in the beams, which acts like a magnetic field along the  $k$ -vectors ( $\hat{x}$  and  $\hat{y}$  in this case) is orthogonal to  $\vec{B}$ . Moreover, the vector shift terms caused by time-phase and intensity imbalance go as the cross-product of the two polarization vectors; for our case, we chose the polarizations in the  $y - z$  plane so that the vector shift term spins along  $\hat{x}$ , which is also orthogonal to  $\vec{B}$ . This configuration was found experimentally to give the smallest vector shifts, and hopefully we have argued convincingly why it is so.

As a demonstration of the effectiveness of these techniques, we compared the measured splitting between the two  $\pi$  transitions in a 2D lattice to those in a 1D lattice. The result of +15(14) mHz showed a slightly larger splitting for the 2D case, but not fully resolved. This is a good indication that the vector shift in a 2D lattice can well-controlled, and gives hope that the same could be true for a 3D lattice as well.

## Chapter 5

### Cold Collisions of Lattice-bound Fermions

As discussed Sec. 1.4 and Sec. 2.3, one key advantage to lattice clocks based on odd isotopes (rather than even isotopes) is the hyperfine quenching of  $^3P_0$ , which naturally enables laser excitation of the  $^1S_0 \rightarrow ^3P_0$  transition. While the hyperfine structure also introduces new complexities associated with optical pumping effects and lattice polarization sensitivities, it currently seems unlikely that these effects will limit the ultimate performance of odd-isotope-based lattice clocks. A second advantage that odd isotopes possess is that they follow fermionic quantum statistics, which potentially can be harnessed to limit atom-atom interactions as discussed below. In other atomic clocks, atom-atom interactions give rise to density-dependent frequency shifts [14, 189, 190, 5, 191]. Because these shifts tend to increase with more atoms, one faces a trade-off between high signal-to-noise (Sec. 2.4) and systematic uncertainty [5]. In lattice clocks, the tight spatial confinement causes the atomic density to be quite high for multiply-occupied lattice sites (see Appendix A), so cold collisions, if left unchecked, can pose a limit to the ultimate accuracy of lattice clocks.

To limit interactions in lattice clocks, it was proposed to use a sample of ultracold, spin-polarized fermions as the atomic standard [192, 42]. This scheme could allow interactions to be very small by freezing out  $p$ - and higher partial-wave contributions while exploiting quantum statistics to prevent  $s$ -wave collisions [193]. That is, identical fermions cannot collide via even-partial-wave collisions (e.g.,  $s$ -,  $d$ -, etc.) because they would have the improper symmetry, and it is straightforward to prepare a sample of identical fermions by spin-polarizing the atoms to a single nuclear spin state. On the other hand, any spherical wave contributions higher than  $s$ - must

overcome the centrifugal barrier between the two atoms; for Yb, the  $p$ - and  $d$ -wave barrier heights are expected to be 30-45  $\mu\text{K}$  and 160-240  $\mu\text{K}$ , respectively, based on calculations of  $C_6$  van der Waals coefficients [194]<sup>1</sup>. Despite these suppression mechanisms, collision shifts have nonetheless been measured in fermionic lattice clocks, both in the  $^{87}\text{Sr}$  lattice clock at JILA and in the  $^{171}\text{Yb}$  system at NIST. In this chapter, we will look at the experiments used to identify, understand, and control these collisional shifts, along with the theoretical work that has accompanied the measurements to provide deeper insight.

These efforts to understand and control the cold collisions are expected to benefit other applications with alkaline-earth atoms beyond lattice clocks. For example, many published proposals for quantum simulation of many-body Hamiltonians [196, 197, 198, 199, 200] and for quantum information processing [201, 202, 203, 204, 205] exploit the rich physical structure of these two-valence electron atoms. Specifically, the decoupling of the nuclear spin from the electronic state ( $\vec{I} \cdot \vec{J} = 0$ ) and the long-lived metastable states  $^3P_0$  and  $^3P_2$  make these atoms attractive candidates for the mentioned applications. In these cases, atom-atom collisions can be a key feature (rather than the complication they are in atomic clocks), possibly useful for creating quantum gates and entangling particles. However, little is known about the relevant scattering parameters in these systems, so perhaps by exploring the collisions in the lattice clocks we can provide valuable information to those other applications.

## 5.1 Preliminary work

Our first measurements of the  $^{171}\text{Yb}$  collision shift were made in a 1D lattice using Rabi spectroscopy. The shifts were measured by varying the number of atoms trapped in the lattice and looking for changes in the Yb clock frequency relative to the Ca optical clock.<sup>2</sup> To systematically study the shift, we varied the relative balance between ground and excited atomic populations. In

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<sup>1</sup>  $V = -C_6/R^6$  gives the long-range dipole-dipole interaction between atoms of separation  $R$ ; adding the centrifugal barrier  $V_l$  for a given partial wave  $l$ , we can then find the height of the barrier of the combined potential as described in [195].

<sup>2</sup> This type of comparison requires an optical frequency comb to span the large frequency gap between Ca and Yb. See Ch. 7 for more details.

Fig. 5.1(a), we plot the measured collision shift (normalized to a typical density of  $\rho_0 \approx 10^{11}/\text{cm}^3$ ) as a function of the final excitation fraction achieved after the long Rabi pulse. The excitation fraction was changed by varying the detuning used to lock to the resonance, while the atom number was varied with slowing beam power [43]. Panel (b) of the same figure shows a few measurements taken in a 2D lattice, again with Rabi spectroscopy.

Having measured non-zero collision shifts, we conclude that either the Fermi suppression breaks down (presumably because the atoms are not truly indistinguishable particles), or the collisional energy of the atoms ( $10 - 15 \mu\text{K}$ ) is sufficiently large for the atoms to tunnel through the  $p$ -wave barrier. We can consider these interactions with a mean-field model. The equations for  $s$ - and  $p$ -wave shifts are [206, 128, 207]:

$$\Delta\nu_s = \frac{2\hbar}{m} G^{(2)} a_{eg} (\rho_g - \rho_e) \quad (5.1)$$

$$\Delta\nu_p = \frac{\pi\hbar}{m} \langle k_T^2 \rangle [b_{gg}^3 \rho_g + b_{ee}^3 \rho_e + b_{eg}^3 (\rho_g - \rho_e)] \quad (5.2)$$

with  $m$  the atomic mass,  $\rho_e$  the density of excited atoms,  $\rho_g$  the density of ground state atoms, and  $k_T$  the thermal de Broglie wavenumber.  $a$  and  $b$  are the  $s$ - and  $p$ -wave scattering lengths, and the subscripts  $g$  and  $e$  denote the type of interaction:  $gg$  for collisions between two ground state atoms,  $ee$  for two excited state atoms, and  $eg$  for one ground and one excited.  $G^{(2)}$  is the two-body correlation function, which summarizes the quantum statistics of the colliding pair. For identical fermions,  $G^{(2)} = 0$  and collisions due not occur, while  $G^{(2)} = 1$  for fully distinguishable fermions. Examining Eq. 5.1 and 5.2, we can highlight three important differences between them:

- i)  $G^{(2)}$  is present only for the  $s$ -wave equation because quantum statistics places no restriction on  $p$ -wave collisions.
- ii)  $gg$  and  $ee$  collisions are excluded for the  $s$ -wave case because two atoms in the same electronic state are identical<sup>3</sup>

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<sup>3</sup> provided they are also in the same nuclear state, which is the case considered here

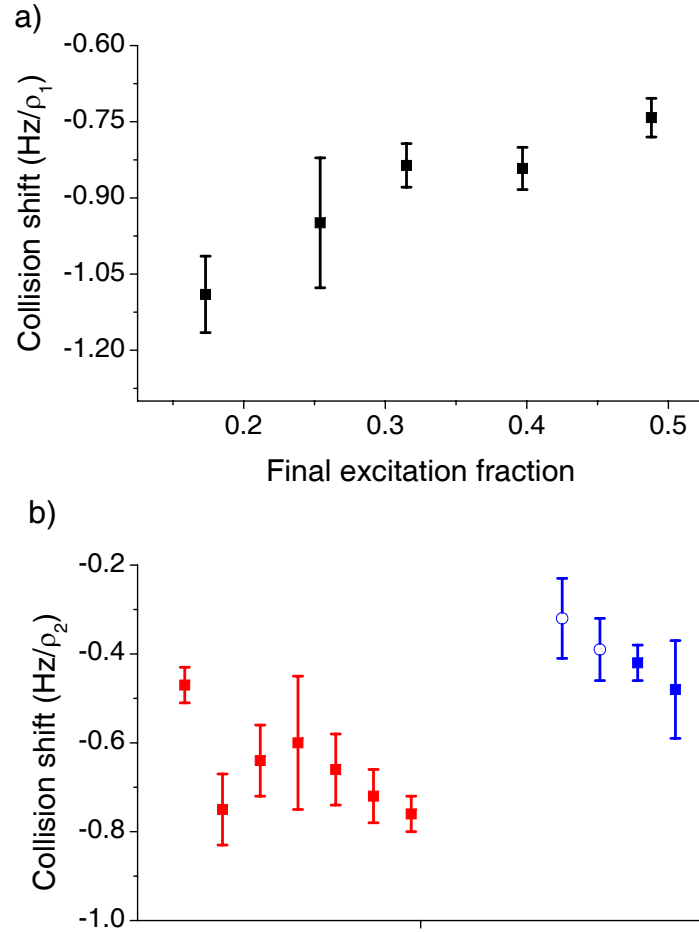


Figure 5.1: a) Measured collision shift versus final excitation fraction for Rabi spectroscopy of 1D lattice atoms. b) A few measurements for 2D confined atoms, using crossed (red) and matched (blue) polarizations. Filled (open) squares denote measurements where the lattices were offset in frequency by 2 (160) MHz. Here the excitation fraction was chosen at its maximal value near 0.6.



iii) Finally, the temperature dependence of  $p$ -wave collisions is included in  $k_T = \sqrt{2\pi m k_B T}/\hbar$  with  $k_B$  the Boltzmann constant, while  $s$ -wave collisions have no such dependence.

As mentioned above,  $s$ -wave collisions can only occur if the fermionic particles are at least partially distinguishable, allowing  $G^{(2)}$  to deviate from 0. In Ref. [128], the JILA group studying fermionic Sr found that excitation inhomogeneity (see Sec. 2.2) does just this. As different atoms, which are Maxwell-Boltzmann distributed throughout the motional states of the lattice, are excited on the clock transition at different rates, their internal states become non-identical, and collisions are enabled [128, 129, 206, 208, 209, 210].

Returning to the data in Fig. 5.1(a), can we now identify which type of interaction gives the measured collision shift? Unfortunately, we were not able to do so with only these initial measurements. We can definitively rule out a  $p$ -wave  $gg$  interaction thanks to published work showing the ground state scattering length to be negligibly small [211]. However,  $a_{eg}$ ,  $b_{eg}$ , and  $b_{ee}$  are all completely unknown. Moreover, while the  $s$ - and  $p$ -wave shifts have very different dependence on temperature and excitation inhomogeneity, a proper treatment requires integrating the shifts over all the pairwise combinations of motional states and integrating over the time evolution of Rabi spectroscopy (including the dependence upon laser detuning). Finally, the mean-field equations above may not be accurate, perhaps due to many-body effects [208] or invalid initial assumptions [209]. All this is to say that the data taken with Rabi spectroscopy could be consistent with either type of interaction, and more work (both experimental and theoretical) was needed to identify the dominant interaction.

In what follows, we show results using two-pulse Ramsey spectroscopy [212] to probe the collision shift. Provided the pulse durations  $t_{1,2}$  are short compared to the dark time between pulses  $T$ , the vast majority of the collisions occur while the atomic population is not being driven by the laser field. This simplifies the analysis by removing the time- and laser-detuning-dependence of the excitation from the collisional dynamics. Furthermore, the Ramsey scheme offers the possibility to explore proposals for cancelation of the cold collision shift by tailoring the Ramsey pulses [209].

In addition to measurements of the collision shift with atoms confined in a one-dimensional (1D) optical lattice, we also show results from a two-dimensional (2D) lattice, which offers several benefits. First, with strong confinement in all but one dimension, the collisions can be treated with an effective 1D model. Second, the higher number of lattice sites in a 2D lattice reduces the overfilling (i.e., many atoms per site). Finally, the 2D lattice yields stronger interactions at any lattice sites that are doubly occupied, thereby offering a different parameter space to explore.

Even with the simplifications afforded by the Ramsey technique applied to a 2D lattice experiment, the collisional dynamics are still complicated enough to require a more sophisticated theoretical model to uncover the relevant physics. To that end, in the next section we consider a more powerful model that was developed in the context of many-body physics, but applied here to the case of two fermions. In section 5.3 we use this model to fit collision shift data taken with Ramsey spectroscopy in both 1D and 2D lattices.

## 5.2 Two-atom spin model

Here we consider two fermionic atoms occupying the same nuclear spin state and interacting via  $s$ -wave and  $p$ -wave. The two atoms are confined in one site of a 2D lattice and occupy the lowest vibrational band of the lattice. In the weakly confined direction (along the “tube”), the atoms see a harmonic potential with trap frequency  $\omega_z$  and occupy modes  $n_1$  and  $n_2$ . The atoms have internal states  $|g\rangle$  and  $|e\rangle$ , and these states experience identical trapping potentials from the lattice. We could analyze the interactions in the individual atoms’ basis states; however, we instead choose the singlet-triplet basis because the interactions are diagonal in this basis. The triplet states ( $|gg\rangle$ ,  $|ee\rangle$ ,  $(|eg\rangle + |ge\rangle)/\sqrt{2}$ ) are symmetric under particle exchange, while the singlet state  $(|eg\rangle - |ge\rangle)/\sqrt{2}$  is antisymmetric. Because spin-polarized fermions are in a symmetric nuclear state, quantum statistics dictates that the triplet states interact by odd-partial-wave while the singlet interacts via even-partial wave.

The atom’s two internal levels are couple by a laser field with wavevector  $\vec{k} = k_Y \hat{Y} + k_Z \hat{Z}$  and detuned from the atomic transition frequency by  $\delta$ .  $k_Z$  is small but non-zero even when  $\vec{k}$  is precisely

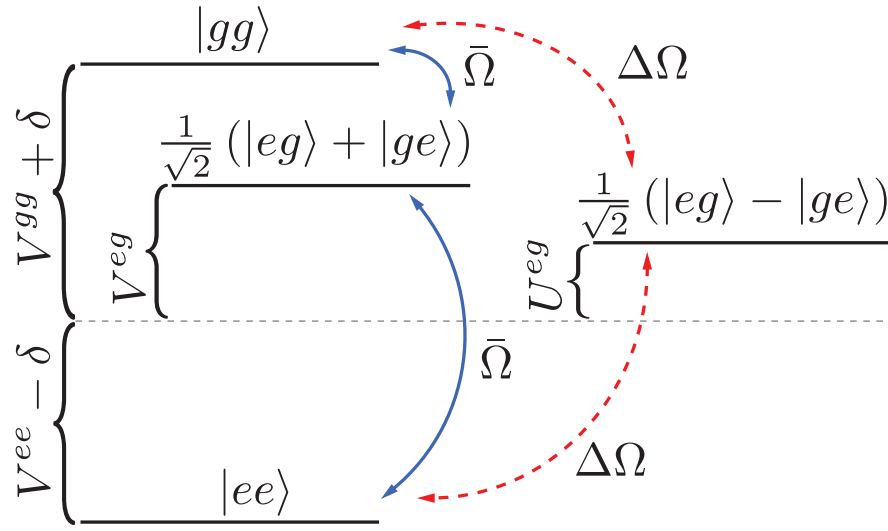


Figure 5.2: Illustration of Eq. 5.3 in the singlet-triplet basis, with  $s$ - and  $p$ -wave interaction terms  $U$  and  $V$ , respectively.

aligned along one of the lattice directions due to the finite wavefront curvature of the lattice beam at its waist. The laser field drives the transition at a rate  $\Omega(n) = \Omega_0 L_n(\eta_Z^2) L_0(\eta_Y^2) e^{-(\eta_Y^2 + \eta_Z^2)/2}$ , with  $\eta_i = k_i \sqrt{\frac{\hbar}{2m\omega_i}}$  the Lamb-Dicke parameter along the  $i$  direction,  $\Omega_0$  the bare Rabi frequency, and  $L_n$  the Laguerre polynomial.  $m$  is the atom mass.

For the two atoms under consideration (labeled  $a$  and  $b$ ), we can define average and difference Rabi frequencies:  $\bar{\Omega} = (\Omega_a + \Omega_b)/2$  and  $\Delta\Omega = (\Omega_a - \Omega_b)/2$ . The atoms are spectroscopically probed using a Ramsey pulse sequence: two pulses of duration  $t_1$  and  $t_2$ , spaced by a dark time of duration  $T$ . The Hamiltonian describing the light-atom interaction and the collisional dynamics is depicted in Fig. 5.2 and is written in the rotating frame and the singlet-triplet basis as

$$H = \begin{pmatrix} \delta + V^{gg} & 0 & \bar{\Omega}/\sqrt{2} & \Delta\Omega/\sqrt{2} \\ 0 & -\delta + V^{ee} & \bar{\Omega}/\sqrt{2} & -\Delta\Omega/\sqrt{2} \\ \bar{\Omega}/\sqrt{2} & \bar{\Omega}/\sqrt{2} & V^{eg} & 0 \\ \Delta\Omega/\sqrt{2} & -\Delta\Omega/\sqrt{2} & 0 & U^{eg} \end{pmatrix}. \quad (5.3)$$

The terms  $U^{\alpha\beta}$  and  $V^{\alpha\beta}$  give, respectively, the  $s$ - and  $p$ -wave interactions between an  $\alpha = \{g, e\}$  and a  $\beta = \{g, e\}$  atom occupying motional states  $n_1$  and  $n_2$ . For simplicity, we ignore interactions during the pulses, which is well-justified provided the following: i) the pulses are short compared to the dark time ( $t_{1,2} \ll T$ ), and ii) the mean collision energy is much smaller than the Rabi frequency ( $U, V \ll \bar{\Omega}$ ). With this simplification, the number of atoms excited after the first pulse is

$$N_{n_1, n_2}^e(t_1) = 1 - \cos(\bar{\Omega} t_1) \cos(\Delta\Omega t_1), \quad (5.4)$$

During the dark time, the Hamiltonian is diagonal and each state acquires just a phase shift. After the second pulse, we recover Ramsey fringes with a frequency shift. Specifically, the excited state population is

$$N_{n_1, n_2}^e(t_1, t_2) = A_{n_1, n_2} + \mathcal{N}_{n_1, n_2} \cos[(\delta - 2\pi\Delta\nu_{n_1, n_2})T], \quad (5.5)$$

with  $A_{n_1, n_2}$  an overall offset,  $\mathcal{N}_{n_1, n_2}$  the fringe amplitude, and  $\Delta\nu_{n_1, n_2}$  the frequency shift. These quantities can be computed analytically, and the full solutions can be found in [213].

In the 2D lattice system an array of isolated tubes is populated with mainly one and two atoms per tube. If  $N_0$  tubes are singly occupied and  $N_1$  tubes doubly occupied, we can write the excitation population as

$$N_{n_1, n_2}^e(t_1, t_2) = \tilde{A}_{n_1, n_2} + \cos[\delta T] (\mathcal{A}_{n_1, n_2}^1 + \mathcal{A}_{n_1, n_2}^2) + \sin[\delta T] \mathcal{B}_{n_1, n_2}, \quad (5.6)$$

and the collisional frequency shift is given by

$$\langle \Delta \nu \rangle_T = \frac{\arctan \left( \frac{\langle \mathcal{B}_{n_1, n_2} \rangle_T}{\langle \mathcal{A}_{n_1, n_2}^2 + \mathcal{A}_{n_1, n_2}^1 \rangle_T} \right)}{2\pi T}, \quad (5.7)$$

with  $\langle \rangle_T$  denoting a thermal average.

We expect Eq. 5.7 to correctly describe the physics of the 2D lattice experiment, provided we numerically calculate the appropriate thermal average over all possible vibrational modes  $\{n_1, n_2\}$ . But, in the 1D lattice, each site is populated by many atoms; as a result, the two-atom model is not directly applicable because the spin model is no longer diagonal in the collective spin basis [208]. However, in the weakly interacting regime, a mean-field picture that approximates the many-atom interactions by a sum of pairwise interactions provides a fair description. Thus we use the two-atom Hamiltonian with temperature-dependent, effective interaction parameters to model the multi-atom case.

While the full analytical solution is cumbersome [213], we gain insight by separately considering  $p$ - and  $s$ -wave interactions in a limiting case. For  $\Delta\Omega = 0$ ,  $t_1 = t_2$  and weak interactions  $V^{\alpha, \beta} T \ll 1$  we obtain the simple expression

$$\Delta \nu_p \sim \frac{V^{ee} - V^{gg} + (2V^{eg} - V^{ee} - V^{gg}) \left( \frac{N_g - N_e}{2} \right)}{4\pi}, \quad (5.8)$$

with  $N_g$  and  $N_e$  the ground and excited atom populations after the first pulse<sup>4</sup>. This expression is analogous to the one obtained for non-condensate bosons [207] and can be understood as the difference in chemical potential of the two components. In this simple limit the shift is independent

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<sup>4</sup> Note that  $(N_g - N_e)/(N_g + N_e) = \cos(\bar{\Omega} t_1)$ .

of the dark time. Again considering weak interactions ( $U^{eg}T \ll 1$ ) and small inhomogeneity we find the  $s$ -wave shift to be [208, 209]

$$\Delta\nu_s \sim \left( \frac{\sin(\Delta\Omega t_1)}{\sin(\bar{\Omega} t_1)} \right)^2 \frac{U^{eg}(N_g - N_e)}{4\pi}. \quad (5.9)$$

The above equations bear strong resemblance to the mean-field equations (Eq. 5.1-5.2), providing a good consistency check into the validity of the model. But outside of the weak interaction and small inhomogeneity limits, the collisional dynamics are more complex, and this model has the potential to uncover new physics that goes beyond the mean-field picture.

### 5.3 Identifying $p$ -wave collisions

#### 5.3.1 Collision shift as a function of excitation fraction

Returning to the Yb experiment but now with Ramsey spectroscopy, we first considered the collision shift as a function of excitation fraction (i.e., the fraction in  $^3P_0$  during the dark time). The excitation fraction was varied by changing the RF power to the AOM that turned on the Ramsey pulses, thus changing the Rabi frequency. The measured shifts with 1D and 2D lattices are shown in the blue and red points in Fig. 5.3(a) and (b). Here, the pulse duration is  $t_1 = t_2 = 1$  ms, and the dark time is  $T = 80$  ms. For these measurements, approximately 25000 atoms at temperature  $\mathcal{T} \sim 10$   $\mu$ K are trapped in the 1D lattice, which gives an estimated density of  $\rho_1 = 3 \times 10^{11}/\text{cm}^3$  and an average of 20 atoms per site. In the 2D lattice, we estimate that 25 % of the  $\sim 7000$  atoms are in doubly-occupied sites, for which the effective density is  $\rho_2 = 4 \times 10^{12}/\text{cm}^3$ , and fewer than 4 % of the atoms are in sites with more than two atoms (Appendix A.2). As discussed in Sec. 4.4, we offset the frequencies of the two lattice beams by 2 MHz using acousto-optic modulators (AOMs), preventing any line-broadening from the vector Stark shift [41, 138, 116, 43]. Atoms not fully confined by the 2D lattice are removed by separately turning off each lattice for 10 ms. With the atoms loaded in either a 1D or 2D lattice, we spin-polarize as discussed in Sec. 3.3; impurity in the spin-polarization is  $\leq 1$  %.

The collision shift is found by repeatedly measuring the frequency offset between high- and

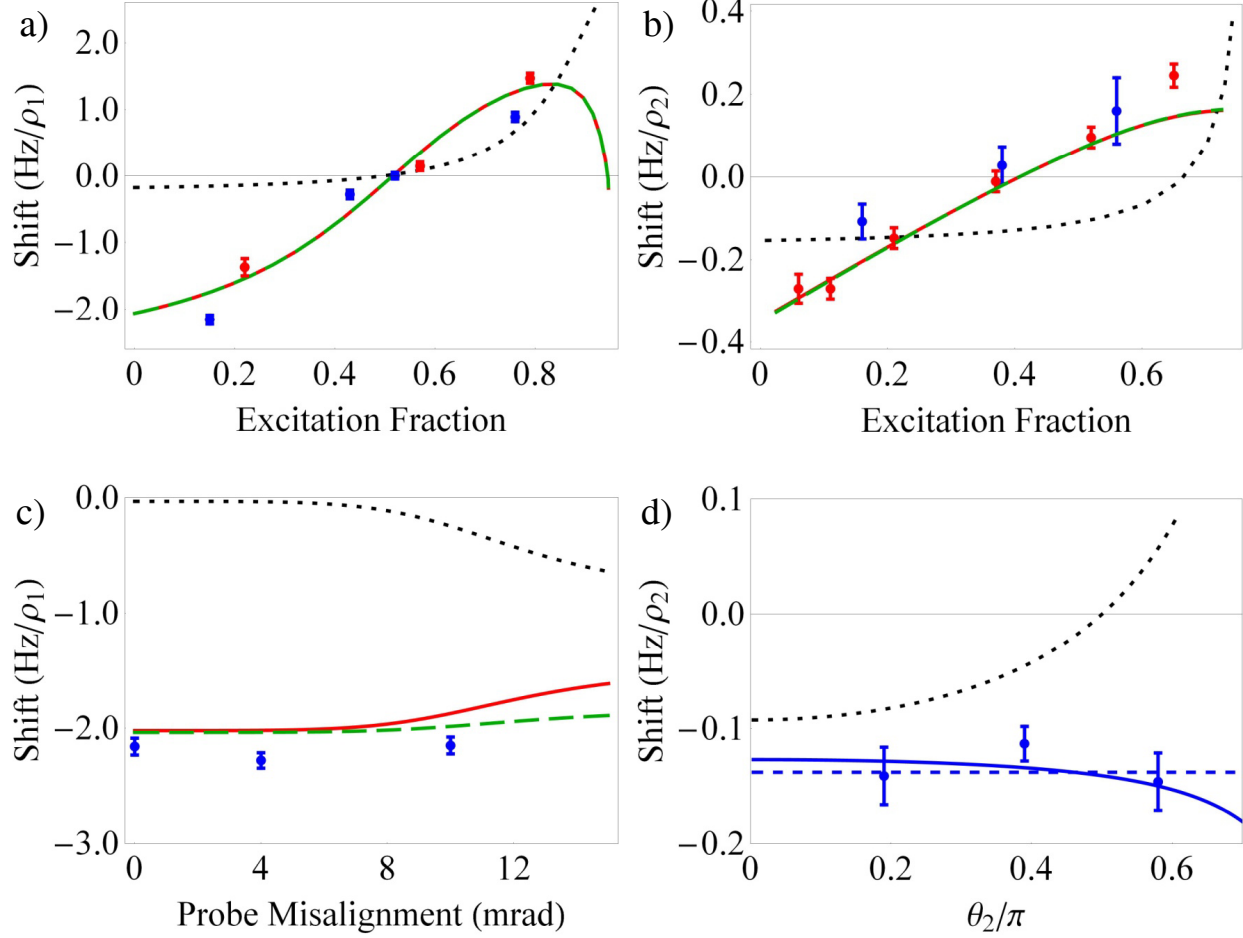


Figure 5.3: (a) Collision shift vs excitation fraction, 1D lattice. Blue (red) points show experimental measurements in a vertical (horizontal) lattice with temperature  $\mathcal{T} \sim 10 \mu\text{K}$  and  $\langle \Delta\Omega/\Omega \rangle_{\mathcal{T}} = 0.2$ . Dashed black line gives an  $s$ -wave-only fit ( $\langle U^{eg} \rangle_{\mathcal{T}} = -2\pi \times 3.0 \text{ Hz}$ ) from the mean-field model. Solid red line gives a  $p$ -wave-only fit with  $\langle V^{eg} \rangle_{\mathcal{T}} = 10\langle V^{ee} \rangle_{\mathcal{T}} = -2\pi \times 2.2 \text{ Hz}$ . Long-dashed green line adds to this a small  $s$ -wave component ( $\langle U^{eg} \rangle_{\mathcal{T}} = -2\pi \times 1.2 \text{ Hz}$ ). (b) Collision shift vs excitation fraction, 2D lattice. Blue (red) points probe along the vertical (horizontal) direction. Dashed black line is an  $s$ -wave-only fit with  $a_{eg}^- \approx -25 a_0$  ( $a_0$  the Bohr radius); solid red line is a  $p$ -wave-only fit with  $b_{eg} \approx -74 a_0$  and  $b_{ee}^3 = 0.1b_{eg}^3$ . The long-dashed green line adds to this a small  $s$ -wave interaction  $a_{eg}^- = -25 a_0$ . We emphasize that these are not necessarily accurate determinations of the scattering lengths since their values depend on the spatial distribution of the atoms in the 2D lattice, which is not well characterized. (c) Collision shift vs probe misalignment angle (vertical 1D lattice) for constant excitation fraction 0.12. Using the same parameters as (a), the dashed black line gives an  $s$ -wave-only fit, solid red line gives a  $p$ -wave-only fit, and the long-dashed green line has  $s$ - and  $p$ -wave terms. In the well-aligned case (0 mrad) there is a residual effective misalignment of  $\sim 5 \text{ mrad}$  due to the imperfect overlap between lattice and probe beams. (d) Measured 2nd pulse dependence of the collision shift (2D lattice, blue points) and expected dependences for  $s$ -wave collisions (black dashed) and  $p$ -wave collisions (solid blue). Dashed blue gives the  $p$ -wave shift in the absence of inhomogeneity.

low-density clock operations relative to the ultrastable optical cavity. We interleave high- and low-density clock conditions, each with its own set of integrators to lock the clock laser to the atomic transition and to average over both  $m_F = \pm 1/2$  spin states. The collisional frequency shift is found by looking at the difference of the correction signals applied to the AOM divided by the difference in atom number, which is typically varied by changing the power to the 399 nm slowing beam that opposes the atomic beam<sup>5</sup>. These interleaved measurements have an instability of  $\leq 1.5 \times 10^{-15}/\sqrt{\tau}$ , for averaging time  $\tau$  in seconds, allowing statistical error bars of  $\sim 20$  mHz in just 2000 s.

For the 2D lattice the black dashed and solid red curves give the numerically calculated shift using the  $s$ -wave scattering length ( $a_{eg}^-$ ) and  $p$ -wave scattering volumes ( $b_{eg}^3$  and  $b_{ee}^3$ ) as fitting parameters. ( $b_{gg}$  is taken to be zero, consistent with prior measurements [211]). For the 1D lattice, the curves are calculated from the mean-field approximation with the effective interaction parameters, which are required to be roughly consistent with those used for the 2D lattice calculations, varied for fitting. As shown in the figure, the  $p$ -wave interaction provides a much better description of the experimental data, as the shift induced by pure  $s$ -wave collisions is generally too small and does not exhibit the correct dependence on the excitation fraction. The shifts go through zero near an excitation fraction of 0.51 in the 1D lattice and 0.4 in the 2D lattice. Zero-crossings near 0.5 are readily understood if  $V^{eg}$  dominates (see Eq. 5.8): by creating equal partial densities of ground and excited atoms ( $N_g = N_e$ ), the energy shift on the two clock levels is the same, and the net shift is canceled. Operation of the clock at this zero-crossing could substantially improve the performance of the Yb system (see Sec. 5.6). The deviation from a zero-crossing at exactly 0.5 in the 1D case is consistent with a small  $ee$  interaction ( $V^{ee} \approx 0.1V^{eg}$ ). The best fit, as shown in the figure, gives  $b_{eg} \approx -74 a_0$  with  $a_0$  the Bohr radius, but this is not necessarily an accurate determination of the scattering length, since the result depends on the spatial distribution of the atoms in the 2D lattice, which is not well characterized.

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<sup>5</sup> The atom number can also be reduced by shortening the time that the slowing light illuminates the atomic beam.



### 5.3.2 Role of excitation inhomogeneity

To further rule out  $s$ -wave interactions, we misaligned the probe beam to couple more strongly to the weak confinement axis of the lattice trap as shown in Fig. 5.3(c). Doing so introduces greater excitation inhomogeneity from the Ramsey pulse (in this case, up to a factor of 2.4) because the atoms are not tightly confined along this axis [128]. We expect the  $s$ -wave shift to depend quadratically on the inhomogeneity, yet the frequency shifts show no change. This insensitivity is well explained by  $p$ -wave interactions, which depend only weakly on inhomogeneity at these levels (decreasing slightly as more population transfers to the singlet state). A small but non-zero  $s$ -wave interaction could balance this effect and may help explain the complete lack of dependence, as shown in the theory curves in the figure. The green long-dashed lines in Fig. 5.3(a,b) also show that adding a small but non-zero  $s$ -wave interaction is consistent with the observed collision shifts. Still, all of these considerations indicate that  $p$ -wave interactions play the dominant role in the cold collisions of  $^{171}\text{Yb}$ .

We also briefly looked for a dependence on the parameters of the second Ramsey pulse. For a fixed first pulse area, we varied the 2nd pulse time and hence its pulse area. No dependence was observed (Fig. 5.3(d)), which is consistent with the model prediction for  $p$ -wave interactions. By contrast,  $s$ -wave collision shifts have been predicted to possess a strong dependence on the 2nd pulse area [209], and this prediction is consistent with two-atom model presented here. The different behavior between  $s$ - and  $p$ -wave collisions seems to be a result of the fact that the  $p$ -wave-interacting triplet state ( $|eg + ge\rangle$ ) is driven much stronger than the  $s$ -wave-interacting singlet ( $|eg - ge\rangle$ ) as  $\bar{\Omega} \gg \Delta\Omega$  [214].

### 5.3.3 Additional measurements and considerations

While the above measurements provide clear evidence for  $p$ -wave collisions, we performed a series of additional measurements that supported this conclusion and justified the exclusion of some physical effects not accounted for by the model. Following is a brief discussion of these

measurements.

i) Tunneling

In Ch. 2 we saw that tunneling effects are present in the Yb lattice clock, and considered possible clock errors related to the atomic motion. Tunneling could also be a relevant process in collision physics [209]. We investigated tunneling effects by measuring the shifts for both vertically and horizontally oriented 1D lattices, exploiting gravity-induced suppression of the tunneling rate [131], but we observed no change in the data (Fig. 5.3(a)). We estimate the tunneling rate, thermally averaged over the lowest nine bands of the 1D horizontal lattice, to be several hertz. In the vertical 1D lattice and the 2D lattice, this rate is suppressed by more than a factor of ten due to the energy offset between adjacent sites (arising from gravity [131] and the 2D Gaussian beam profile, respectively). However, the two highest bands of the lattice, which are populated with a few percent of the atoms, can have very high tunneling rates (several kilohertz) that are not suppressed by the energy offset. Because of this, the fraction of atoms that can tunnel during the spectroscopic time are 10 %, 5 %, and 10 % for the horizontal, vertical, and 2D lattices, respectively. We do not see any appreciable difference between the shifts measured in the horizontal and vertical lattices and thus conclude that tunneling does not play a significant role in the collision shifts.

ii) Inverted spectroscopy

We measured the shift vs. excitation for atoms initially prepared in the excited state rather than the ground state. To do so, a quick pulse of the clock light excited some of the atoms to  $^3P_0$ , after which the 399 nm probe light heated away remaining ground state atoms. We then proceeded with usual Ramsey spectroscopy. This allowed us to probe the shift at very high excitation fraction, and to check for any contamination from imperfect spin polarization (since any atoms in the opposite spin state were removed with the 399 nm light.) The results of the measurement are shown in Fig. 5.4(a).

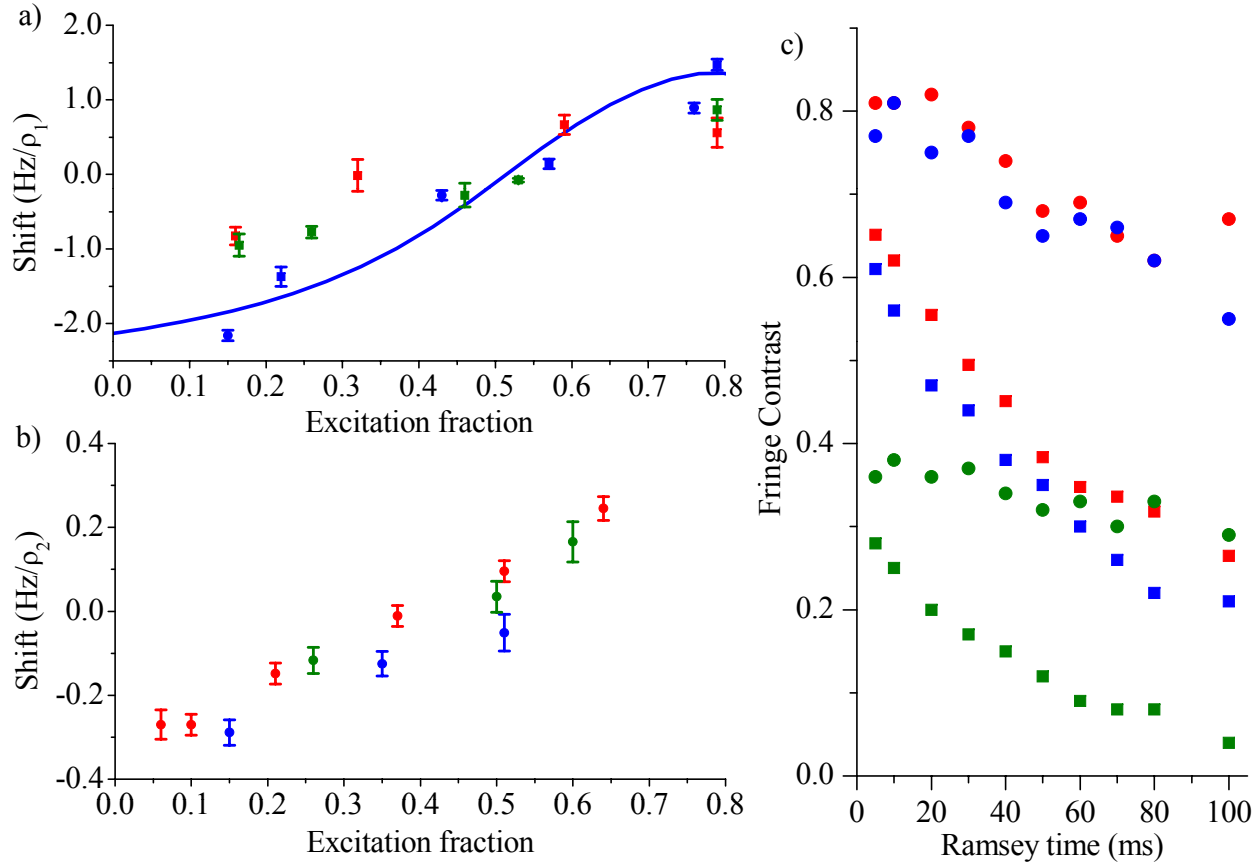


Figure 5.4: a) Here we show the collision shift vs. the excitation fraction in a 1D lattice for inverted spectroscopy (green diamonds) and for an unpolarized sample (red squares). Also shown (blue markers) is the result for typical conditions and the prediction of the model (blue line), both repeated from Fig. 5.3(a). b) Here we plot the measured shift vs. excitation fraction curve in a 2D lattice for three different pulse times. The blue, red, and green colors correspond to  $t_{1,2} = 0.5, 1, 5$  ms. Because no significant dependence on pulse time is observed, we conclude that laser-assisted mode-changing collisions do not play a significant role in the experiment. c) Ramsey fringe contrast vs. Ramsey dark time for 3 pulse areas (red, green, and blue). The dependence of the contrast on atom number is highlighted by measuring each set with high (squares) and low (circles) atom numbers.

### iii) Unpolarized atomic sample

Any degree of imperfect polarization of the nuclear spin state introduces a host of other possible atomic interactions. In  $p$  wave, the  $V_{eg}^-$  interaction, which shifts the singlet state, becomes allowed. Furthermore, distinguishability between different nuclear spin states allows  $s$ -wave interactions  $U_{gg}$ ,  $U_{ee}$ , and  $U_{eg}^+$ . In  $^{171}\text{Yb}$ , both the  $s$ - and  $p$ -wave  $|gg\rangle$  interaction terms are small [211]. However, the remaining interactions can alter the observed collision shift from the spin-polarized case. For this reason, high polarization purity is important for optical lattice clocks. Here, we benefit from the simple structure ( $I = 1/2$ ) of  $^{171}\text{Yb}$  and can readily optically pump to a single spin ground state with 99 % purity. The polarization purity is directly measured by observing the absence of a clock excitation spectrum for the unpopulated spin state.

To quantify the effect of imperfect polarization, we measured the collision shift as a function of excitation for unpolarized atoms (red squares in Fig. 5.4(a)) with equal mixture of both spin states. Since, during spectroscopy, a weak bias field ( $\sim 1$  G) lifts the degeneracy of the  $\pi$ -transitions from the two spin states, here the excitation fraction is defined as that for the particular spin state being resonantly excited, not accounting for the other ‘spectator’ spin state. In general, the measured shifts are smaller than for the spin-polarized case, implying that competing interactions have the opposite sign as those in the polarized case. Notably, the measured zero-crossing in the shift occurs at a lower excitation fraction (around 40 %), leaving a net positive shift at 51 %, where the shift is zero for the spin-polarized case. Based upon these measurements, we determine a 1 % polarization impurity will not affect the shift zero-crossing at a significant level.

### iv) Mode-changing collisions

In the 1D lattice there are two weakly confined directions and multiple atoms per lattice site. Under these conditions, interaction-induced mode-changing collisions, which are not accounted for in our two-atom model [208], have to be included. Our collaborators at JILA studied the

role of those processes by numerical evaluation of a more general multi-mode Hamiltonian and found that it mainly leads to a renormalization of the model parameters. This effect is one more reason why the interaction parameters used to fit the 1D lattice data must be understood as effective parameters, and cannot be related to an absolute scattering length [213, 132].

We use short Ramsey pulses ( $t_{1,2} \sim 1$  ms) to avoid interaction effects during the pulse. But, for pulses shorter than the mean oscillation period in the trap,  $\Omega \gtrsim \omega_i$ , with  $i$  the weakest trap direction, and laser-induced mode-changing collisions are not necessarily suppressed. Nevertheless, we ruled out the relevance of those processes by varying the pulse duration over a factor of ten without observing any substantial modification to the measured collision shifts, as shown in Fig. 5.4(b).

#### v) Contrast decay

In general, the decay of Ramsey fringe contrast with longer Ramsey times is a sign of decoherence between the atom and light fields. But a correlation between this decay rate and the atom number suggests some interesting collisional physics. We looked for, and found, such a correlation by measuring fringe contrast as a function of time for various excitation fractions and different atoms numbers, as shown in Fig. 5.4(c). These measurements were performed with a 1D lattice, where many atoms occupy each lattice site. The observed contrast decay may be a sign of many-body collisional effects [132]. The exact mechanism that causes the contrast to decay is still under investigation, though it likely involves both elastic and inelastic collisional processes. At the highest atom numbers, the decay in contrast could hinder the observation of narrower spectral features as we look to improve the stability of the clock by probing for longer durations. Of course, the atom number can always be reduced if the lack of contrast becomes problematic. Looking ahead the measurements in Sec. 5.6 where we demonstrated cancelation of the collision shift, the relevant parameters were such that the Ramsey fringe contrast was near 30 %, which was more than sufficient for achieving high stability.

vi) Control measurements

To ensure that the measured correlations between clock frequency and atom number are caused by collision effects, we investigated several control measurements. Several are summarized below.

a) Probe pulse power

Instead of alternating between high and low atom number, we toggled between high and low probe pulse power, which gives rise to an apparent variation of atom number. Nonetheless, no shift was observed between the two conditions, which gives confidence that observed collision shifts can be attributed to atomic effects rather some unknown error in signal processing.

b) 3rd pulse power

Again, instead of varying the atom number, we toggled between full and reduced optical power in the 3rd detection pulse (which measures excited state atoms). Doing so largely ruins the normalization and decreases the Ramsey fringe size. No shift was observed between the two conditions, indicating that changes in normalization and fringe size do not introduce a frequency shift.

c) PMT gain

We doubled the gain of the photomultiplier tube that converts fluorescence signals into atom “counts.” Doing so doubles the value of all electrical signals after the PMT. We then measured the collision shift coefficient and found agreement (accounting for the factor of 2 increase in apparent atom number with higher PMT gain).

d) Several ways to change the density

One slightly mysterious effect observed in Yb clock system is that changes in the slowing (and trapping) optical power produce changes in the background signal (i.e. the 2nd pulse fluorescence). Thus, as we change the slowing beam power to alternate the density between high and low, this also produces an unwanted change in the background signal. One might

worry that this is due to cold atoms lingering in the vicinity of the lattice, but outside the lattice trap, and that these atoms somehow cause problems which mask the collisional dynamics. We found that changing the atom number with slowing power, with slowing time (i.e. the amount of time the slowing beam is turned on), and with green cooling parameters (bypassing the first stage of green cooling in favor of a longer second stage) were all effective means for varying the atom number, and each had different effects on the background pulse fluorescence. We separately measured collision shifts using each mechanism to change the density, and found mutual agreement.

## 5.4 Strong interactions

It is interesting to see how collision effects are manifest in a regime of high density and strong interactions (e.g.  $V^{\alpha,\beta}T \geq 1$ ). A key observation revealing the operation of the 2D lattice clock in the regime  $V^{ge}T \gg V^{ee}T \geq 1$  is the zero-crossing of the collision shift at a lower excitation fraction of 0.4, which deviates from the crossing near 0.5 found for weak interactions (Fig. 5.3 and Eq. 5.8). This change occurs due to the nontrivial counterplay between  $V^{ge}$  and  $V^{ee}$  in the strongly interacting regime. The interaction strength also introduces additional dependencies on the dark time. In the weakly interacting regime,  $TV^{\alpha,\beta} \ll 1$  and  $TU^{eg} \ll 1$ , the  $\mathcal{B}$  term in Eq. 5.7 provides the leading contribution, because it exhibits a linear dependence on interactions:  $\mathcal{B} \propto (TV^{\alpha,\beta}, TU^{eg})$ . This results in a  $T$ -independent collision shift. On the other hand, in the strongly interacting regime,  $(TV^{\alpha,\beta}, TU^{eg}) \gg 1$ , both terms  $\mathcal{B}$  and  $\mathcal{A}$  exhibit a nontrivial sinusoidal dependence on the various interaction parameters. This implies that as  $T$  increases, both  $\mathcal{B}$  and  $\mathcal{A}$  exhibit faster but bounded oscillations and therefore, according to Eq. 5.7, on average the shift decays as  $1/T$  [213, 215].

We investigated this experimentally by varying the dark time  $T$  and measuring collision shifts in the 1D lattice (Fig. 5.5(a)), where the shift scales weakly with  $T$ , and the 2D lattice (Fig. 5.5(b)), where the shift is strongly damped towards zero with increasing  $T$ . In panel c) of the same figure, we plot the shift as a function of excitation fraction for several dark times. Together with the

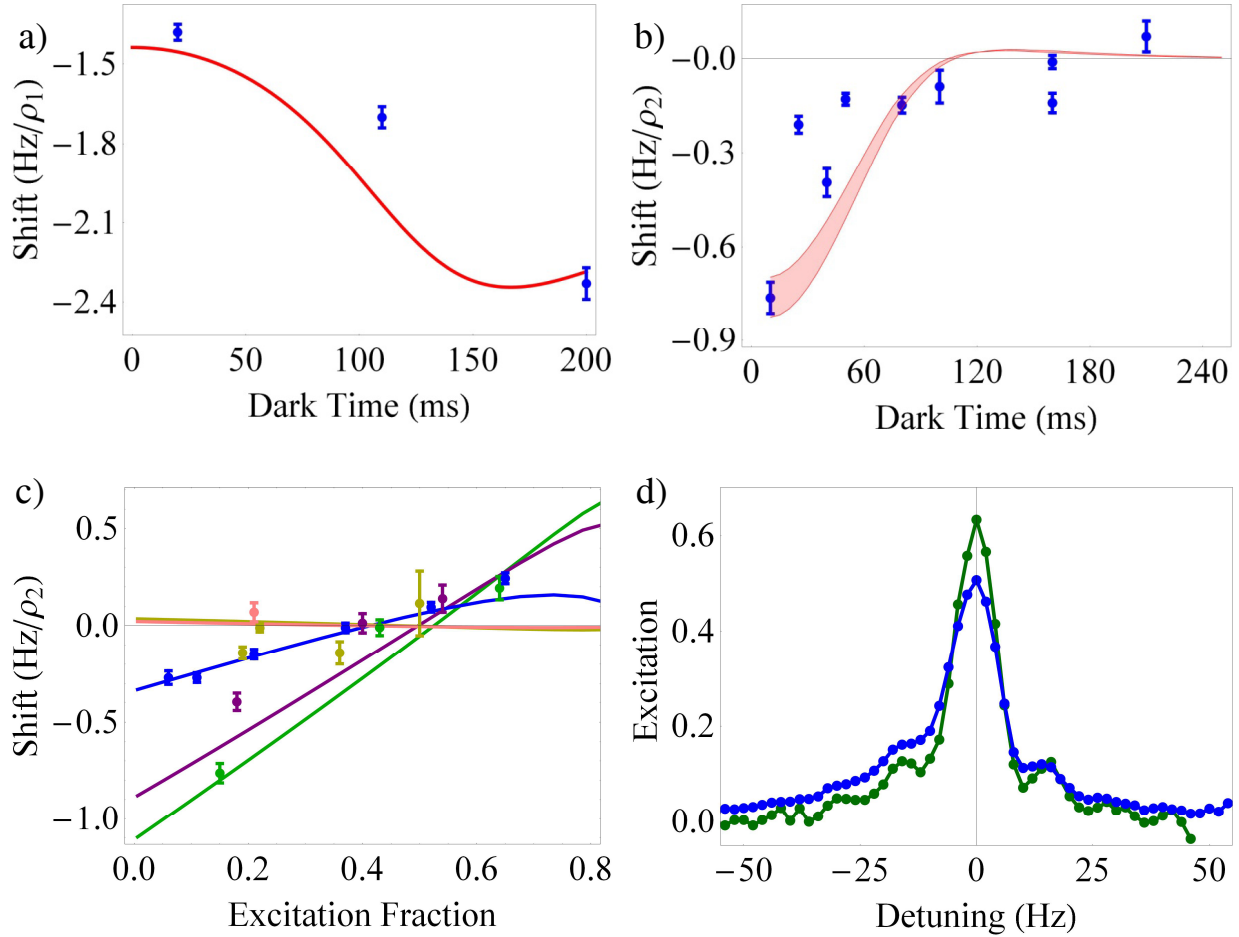


Figure 5.5: (a) Collision shift vs dark time, 1D lattice, for excitation fraction 0.18. Using the same parameters as Fig. 5.3(a), the solid-line gives a fit from the mean-field model. (b) Collision shift vs dark time, 2D lattice, for excitation fraction  $0.19 \pm .03$ . The shift crosses zero due to the periodic dependence of the shift on collisional phase, and is a signature of strong interactions. The model calculations (shaded region) use the same parameters as Fig. 5.3(b) for an excitation fraction range  $0.19 \pm .03$ . c) In the 2D lattice, the shift as a function of excitation exhibits a strong dependence on the dark time. Green:  $T=10$  ms. Purple:  $T=40$  ms. Blue:  $T=80$  ms. Gold:  $T=150$  ms. Pink:  $T=210$  ms. Generally, the shifts are smaller for longer  $T$ . The zero-crossing is also moved away from 0.5. d) Asymmetric Rabi spectrum in a 2D lattice. The blue curve was taken under the highest density conditions, while the green curve was taken with reduced (by a factor of  $\sim 5$ ) density.



theory curves (solid lines), these data reveal a general trend that the shifts decrease with longer Ramsey times; however, the exact point of zero shift can move in a non-intuitive way.

Yet a third signature of strong interactions is significant asymmetry in the clock transition spectrum. In Fig. 5.5(c) we show a Rabi spectrum ( $t = 120$  ms), taken under high density operation in the 2D lattice, which shows an additional feature on the red side ( $\delta < 0$ ) of resonance. This asymmetry is density-dependent and barely observable in the 1D lattice. In the 2D lattice, the interactions are sufficiently strong ( $V^{eg}t \geq 1$ ) to introduce these asymmetric lineshape features beyond the transition linewidth. With yet higher density, it may be possible to spectrally resolve three features, one each for the  $s$ -wave-interacting singlet, the  $p$ -wave-interacting triplets, and the non-interacting atoms in singly occupied lattice sites. Interaction-induced sidebands were recently reported in [216] and may be useful for quantum simulation applications.

## 5.5 Inelastic collisions

Collisions are typically labeled “elastic” and “inelastic” based on whether they conserve kinetic energy. Inelastic collisions are those which convert internal electronic energy into excess kinetic energy. Because the lattice trap depth is 8 orders of magnitude lower than the photon energy of an optical transition, this additional kinetic energy kicks the colliding atoms out of the trap. For that reason, we can study inelastic processes by simply monitoring the number of trapped atoms over time. Collisions between one cold Yb atom and a background gas atom or molecule (notably  $\text{H}_2$  at ultrahigh vacuum) we call one-body loss and model with a simple exponential decay. Collisions between two Yb atoms (at least one of which must be excited out of the ground state) we call two-body loss, and the loss rate is proportional to the square of the density.

We have observed inelastic two-body losses involving both  $^3P_0$ – $^3P_0$  and  $^1S_0$ – $^3P_0$  interactions. With both  $^1S_0$  (g) and  $^3P_0$  (e) populations present, the number density rate equations are:

$$\dot{n}_g(t) = -\Gamma_g n_g(t) - \beta_{eg} n_g(t) n_e(t) \quad (5.10)$$

$$\dot{n}_e(t) = -\Gamma_e n_e(t) - \beta_{eg} n_g(t) n_e(t) - \beta_{ee} n_e(t)^2. \quad (5.11)$$

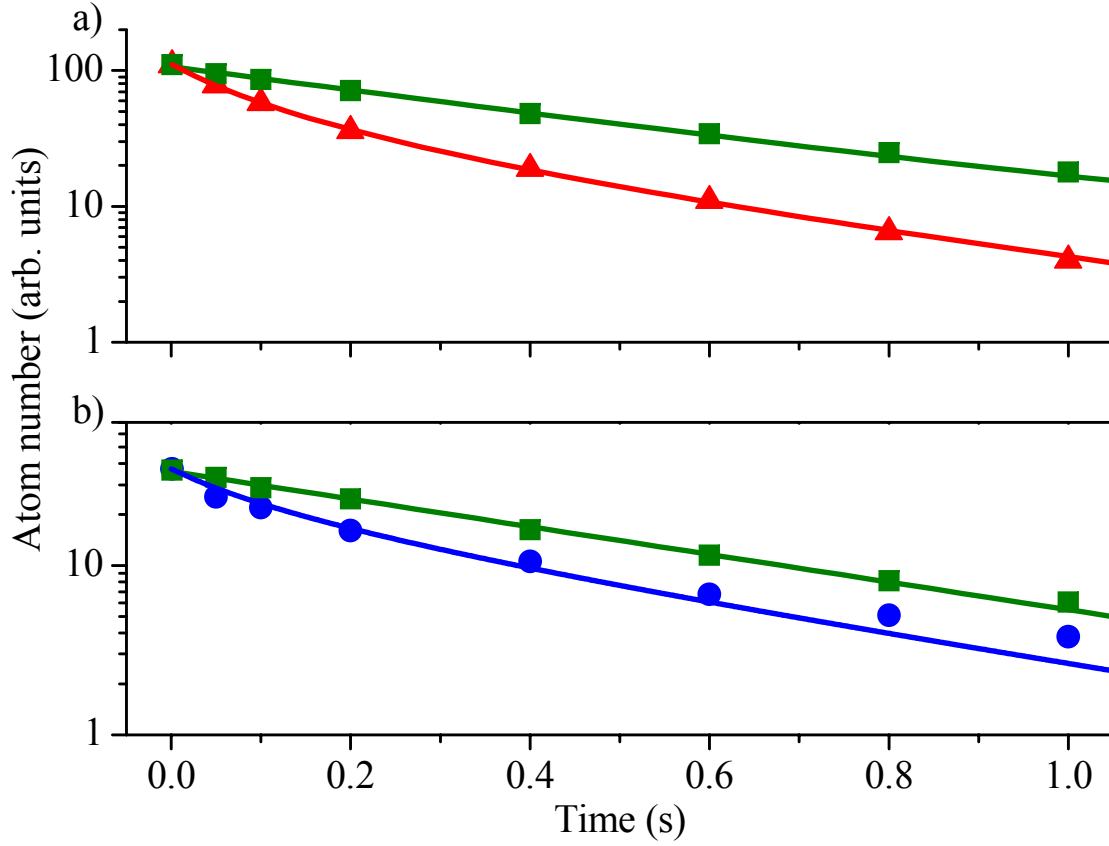


Figure 5.6: a) Ground state trap loss as a function of time (green squares). A one-body loss fit (green line) gives  $1/\Gamma_g = 480$  (20) ms. Also shown is excited state loss (red triangles) and a fit (red line) that includes one- and two-body losses using  $1/\Gamma_e = 520$  (28) ms and  $\beta_{ee} = 5 \times 10^{-11} \text{cm}^3/\text{s}$ . b) Ground state trap loss with (without) excited state atoms are shown in blue (green). The slightly higher loss observed in the former case indicates  $\beta_{eg} = 3 \times 10^{-11} \text{cm}^3/\text{s}$

For a pure state population (either  $n_g$  or  $n_e$ )  $\beta_{eg}$  loss can be ignored. Fig. 5.6(a) shows the trap loss for ground state atoms (green squares). Fitting an exponential decay gives the one-body lifetime of  $1/\Gamma_g = 480$  (20) ms. In the same figure (red triangles) we also show the excited state loss; here, the atoms were excited with a quick pulse of the clock field, after which any remaining  $^1S_0$  atoms were heated away with the 399 nm light. This population experiences stronger decay at the highest density, and good fit requires both one-body ( $\Gamma_e$ ) and two-body ( $\beta_{ee}$ ) losses. To express  $\beta_{ee}$  as an absolute loss rate, we must calibrate the experimental fluorescence signals into absolute atom number, with which we can calculate the atomic density. After integrating over the atoms' spatial extent within a lattice site, as well as across the distribution of occupied sites, we find  $1/\Gamma_e = 520$  (28) ms (consistent with  $\Gamma_g$ , as one might expect) and  $\beta_{ee} = 5 \times 10^{-11} \text{cm}^3/\text{s}$ . Because the process of calibrating the absolute atomic density is challenging, we place a conservative error of 60 % on  $\beta_{ee}$ . This inelastic rate is somewhat larger than those reported for fermionic and bosonic Sr [217, 218, 73]. As with the elastic collisions described earlier in this chapter, inelastic collisions between ultracold, identical fermions must be  $p$ -wave.

For an unpolarized sample of  $^3P_0$  atoms (here with equal  $m_F = \pm 1/2$  populations), interactions between distinguishable atoms also include an  $s$ -wave term, and the loss rate for distinguishable  $^3P_0$  atoms is labeled  $\tilde{\beta}_{ee}$ . The total loss rate for the unpolarized sample, given by the average of  $\beta_{ee}$  and  $\tilde{\beta}_{ee}$ , was found experimentally to be identical (within 10 %) to the polarized case.

For a mixed population of  $^1S_0$  and  $^3P_0$  atoms, we observed additional loss through  $\beta_{eg}$ . Fig. 5.6(b) highlights this by comparing  $^1S_0$  trap loss for two different atomic samples: with (blue) and without (green) the presence of  $^3P_0$  atoms. The additional loss is particularly notable at short times, where both  $^1S_0$  and  $^3P_0$  populations are large. Using the same calibration of atomic density as for  $\beta_{ee}$ , here we find a  $^1S_0$ - $^3P_0$  two-body loss rate at the level of  $\beta_{eg} = 3 \times 10^{-11} \text{cm}^3/\text{s}$ . The  $^3P_0$  population is excited coherently from the  $^1S_0$  state, but due to excitation inhomogeneity, the lossy collisions are between partially distinguishable atoms. The magnitude of the inelastic loss is noteworthy because, at long range, only the  $^1\Sigma_g^+$  ground state (correlating to the  $^1S_0$ - $^1S_0$  state) lies at lower energy than molecular states correlating to a  $^1S_0$  and  $^3P_0$  atom pair and long-range

coupling to this state is spin-forbidden.

One consequence of these inelastic losses is that the excitation becomes time- and density-dependent. This, in turn, alters the balance between the (elastic) collision shifts, and to some extent frustrates our ability to cancel the collision shift by precisely tuning the excitation fraction, as discussed in the following section.

## 5.6 Suppressing the cold collision shift

### 5.6.1 Cancellation in a 1D lattice clock

As shown previously, the collision shift crosses through zero for an excitation (during the Ramsey dark time) near 50 %, and this zero-crossing is the focus of our attention here. We can understand the zeroing of the shift in the separated atom basis as follows: the ground (excited) population of atom  $a$  shifts the excited (ground) state of atom  $b$ , and near 50 % excitation, these shifts are identical. (For  $V^{ee} \neq V^{gg}$  the point of zero shift moves slightly from 50 %.) The collision-shift-cancellation is thus similar to the magic wavelength technique in that it equalizes the shifts on the individual clock levels, leaving zero net shift for each atom. In the singlet-triplet picture, we can also understand the cancellation. Here, the important point is that a symmetric state (i.e. the same population in  $|gg\rangle$  as  $|ee\rangle$ ) is populated during the dark time, after which the second Ramsey pulse's equal coupling terms from the triplet state to  $|gg\rangle$  and  $|ee\rangle$  and opposite detuning dependence (see Eq. 5.3) preserve the symmetry and cancel the shift.

Experimentally, there are two challenges to this effort. First, we must demonstrate an ability to control the excitation over long timescales. In fact, this turned out to be more difficult than expected, as even an active servo loop that maintained the  $\pi$ -polarized component of the clock laser field was insufficient to fix the excitation fraction over several hours<sup>6</sup>. To overcome this problem, we made frequent measurements of the excitation fraction by turning off the second Ramsey pulse and measuring the ground and excited atomic populations after the dark time. These measurements

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<sup>6</sup> Presumably the drift in excitation was caused by slow changes in the clock laser beam alignment or the vacuum viewport birefringence, neither of which are fully and accurately compensated in our control loop.

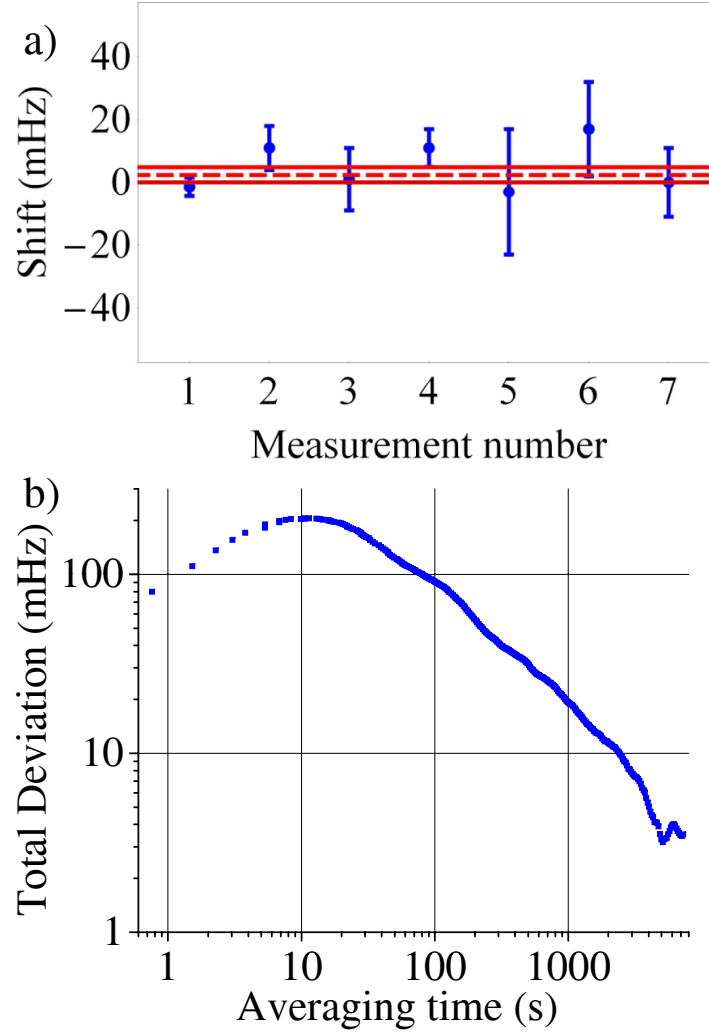


Figure 5.7: By tuning the excitation fraction to 0.51, the net shift is cancelled. In the top figure are 7 measurements of the residual shift at this excitation fraction. Note that measurement number 2 was corrected by  $-5$  ( $2.5$ ) mHz. The lower panel shows the total deviation (a measure of instability) for the data in measurement 1 above. For these data, the density was approximately  $\rho_{1D} = 3 \times 10^{10}$ .

were interspersed between cycles of usual Ramsey spectroscopy. We then slightly adjusted the probe laser power to keep the mean measured excitation fraction constant during each shift measurement.

Second, we must be able to make sufficiently precise measurements of the shift at a given excitation to identify which value cancels the shift. Ideally, we would like to use a very large number of atoms to measure the zero-crossing, then operate the clock with significantly fewer atoms and enjoy a reduced error bar. However, leveraging the shift in this manner is not possible due to the two-body loss processes described previously, which lead to a time-dependent excitation fraction during the Ramsey dark. This, in turn, affects the balance between the  $^1S_0$  and  $^3P_0$  collisionally induced energy shifts. Instead, we chose to measure shifts and to operate the clock at the same atom number density. Specifically, we chose a reduced atom number, one-tenth the maximum, thereby reducing not only the collisional shifts, but also the two-body inelastic losses. The number of quantum absorbers remains well in excess of 1000, in order to accommodate a high signal-to-noise ratio, and the reduced requirements for atom number allowed for shorter loading times and a smaller Dick effect (see Sec. 3.6). At a density of  $\rho_{1D} = 3 \times 10^{10}$ , the excitation fraction over a dark time of  $T = 150$  ms changes by only several percent. We therefore take the dark-time-averaged excitation value to indicate the excitation fraction where the shift is canceled.

The precision of the zero-crossing measurement is given by the clock instability during interleaved measurements of high and low atomic density. Fig. 5.7(b) shows the precision of one such measurement, where we observed a collision shift of -1.4 (3) mHz after 14500 s of averaging. Fig. 5.7(a) shows the result of seven similar measurements, taken sequentially over the course of several weeks and with different measurement durations. For all but one measurement, the mean excitation fraction was controlled to  $51 \pm 0.3 \pm 1.3$  %, where the first uncertainty is the statistical fluctuation in the measured excitation fraction and the second is the systematic uncertainty in the absolute excitation value (with uncertainty contributors including repump efficiency, offsets in the detection system, and excitation decay during spectroscopy). (For data point number two, the excitation fraction was set to 1 % higher; we thus applied a -5 (2.5) mHz correction to the measured collision shift, as determined from the slope of the curve in Fig. 5.3). The weighted mean of the

seven measurements (red lines) is 2.5 (2.4) mHz ( $\chi_{\text{red}}^2 = 1.04$ ). This corresponds to a fractional shift of  $4.8 (4.6) \times 10^{-18}$  of the transition frequency, and demonstrates the smallest measurement of a collision shift in a lattice clock.

We have shown that the cold collision shift can be canceled at the  $5 \times 10^{-18}$  level in a  $^{171}\text{Yb}$  optical lattice clock. The excitation fraction required to achieve this cancelation is compatible with high signal contrast. It is noteworthy that this cancelation is achieved in a 1D optical lattice, where polarization and intensity control at a particular lattice site are simpler than for a 3D lattice implementation, thus enabling finer control of lattice shifts which depend on the vector or tensor polarizability and hyperpolarizability. Moreover, the large trapping volume of the 1D lattice sites generally yields weaker elastic and inelastic interactions at multiple-occupancy sites.

### 5.6.2 Other suppression mechanisms

Other lattice implementations may be suitable for reducing the clock shift at or below the level shown above. In a 2D optical lattice clock, strong interactions can lead to a decay of the collision shift [213, 215]. In particular, longer Ramsey dark times lead to smaller shifts and can reduce the shift dependence on excitation fraction, making it attractive for shift reduction. Care must be taken since, as we have observed both experimentally and theoretically, the interactions can also reduce Ramsey fringe contrast. Alternatively, the 2D lattice system also exhibits a zero crossing in the shift as a function of excitation. However, strong interactions can move the zero-crossing excitation with a nonlinear dependence on interaction strength, and thus the weak interactions of the 1-D lattice may be easier to control.

The 3D optical lattice continues to be an interesting choice [40, 91, 219], where it is expected to be straightforward to achieve high atom number with far less than one atom per lattice site (on average). The small fraction of lattice sites with double occupancy will exhibit very strong interactions. Doubly-occupied sites could also be eliminated using photoassociation losses [219] or directly via the two-body losses observed here. Furthermore, the 3-D optical lattice system may exhibit kinematic suppression of the atomic interactions which yield the shifts [220]. Indeed, these

rich atomic systems will undoubtedly continue to offer many interesting phenomena in 1-, 2-, and 3-dimensional confinement.



## Chapter 6

### A Step Toward $10^{-18}$ : Precise Measurement of the Static Polarizability

#### 6.1 The blackbody radiation shift

Blackbody radiation (BBR) is the physicist's term for the light emitted by matter with non-zero temperature. The white light from an incandescent lightbulb and a red-hot iron in the fire are two well-known examples, though room-temperature blackbody radiation lies in the infrared and goes unnoticed by the human eye. A true blackbody is a perfect absorber at all wavelengths and emits a continuous energy spectrum based on its temperature. Real matter deviates from this ideal case in a manner that can be characterized by the emissivity parameter, a dimensionless quantity comparing the fraction of radiation absorbed by the material to that absorbed by a perfect blackbody. Thus the emissivity of a certain material (at a specific wavelength) is between 0 and 1.

Blackbody radiation affects atomic clocks via the Stark effect. The BBR electric field ( $E$ ) polarizes the atom, and the polarized atom has a small dipole interaction with the field, causing a frequency shift that scales as  $E^2$ . Because the peak of the BBR spectrum is far detuned from any atomic transitions involving either clock state, the BBR shift can be modeled as a d.c. Stark shift with a small dynamic correction (typically of order a few percent) that accounts for the non-static aspect of the shift [221]. We can write the shift as

$$\Delta\nu = -\frac{1}{2}\alpha_{\text{clock}}\langle E^2 \rangle [1 + \eta_{\text{clock}}(T)] \quad (6.1)$$

with  $\langle E^2 \rangle$  the time-averaged intensity of the BBR field,  $\alpha_{\text{clock}} = \alpha_e^{(0)} - \alpha_g^{(0)}$  the difference in static

polarizability between the excited and ground clock states, and  $\eta_{\text{clock}}$  the dynamic correction.<sup>1</sup>

For matter in thermal equilibrium, the absorption and re-emission of BBR fields is governed by the Stefan-Boltzmann law. The time-averaged intensity of the BBR field can be written as [222, 223]

$$\begin{aligned}\langle E^2 \rangle &= \int_0^\infty \frac{8\pi h\nu^3}{\epsilon_0 c^3 \left( e^{\frac{h\nu}{k_B T}} - 1 \right)} d\nu \\ &= \frac{8\pi^5 k_B^4 T^4}{15 c^3 h^3 \epsilon_0}\end{aligned}\tag{6.2}$$

with  $\alpha$  the fine-structure constant and  $T$  the temperature of the blackbody. At room temperature ( $T = 300$  K), the BBR intensity is  $\langle E^2 \rangle \approx (8.32 \text{ V/cm})^2$ .

For all lattice clock atoms including Yb and Sr, knowledge of  $\alpha_{\text{clock}}$  is theoretical, based on relativistic many-body calculations of atomic structure [221, 224, 194]. Generally, these calculations are accurate to within a few percent, but for Yb the uncertainty is larger (10 %), due in part to incomplete knowledge of the role of core excitations [221, 194]. For this reason, in our first evaluation of the Yb clock, the uncertainty associated with the blackbody shift was  $2.5 \times 10^{-16}$  [43]. The BBR shift is thus the largest shift and the largest source of uncertainty in the best-characterized lattice clock systems [1, 43, 49].

In principle, one could accurately determine the polarizability with precise knowledge of energy splittings and line strengths of all the intermediate states that couple to the clock states. Generally, the energy spectrum has been measured with very high accuracy, while the line strengths (including lifetimes and branching ratios) have not. With Sr, it was shown that just four of the low-lying states provide the dominant contribution, and with 0.1 % uncertainty in their contributions,  $\alpha_{\text{clock}}$  could be known to the same level [224]. However, line strengths are generally difficult to measure with high accuracy. A different approach is to measure  $\alpha_{\text{clock}}$  directly by applying an electric field to the atoms and observing the frequency shift produced [225]. With an applied field of 100 V/cm, the associated shift is 300 – 400 Hz, easily measured with a state-of-the-art optical clock. More challenging, though, is to create an electric field that is known with high accuracy.

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<sup>1</sup> State-specific values help to define  $\eta_{\text{clock}} \equiv (\eta_e \alpha_e^{(0)} - \eta_g \alpha_g^{(0)}) / \alpha_{\text{clock}}$ .

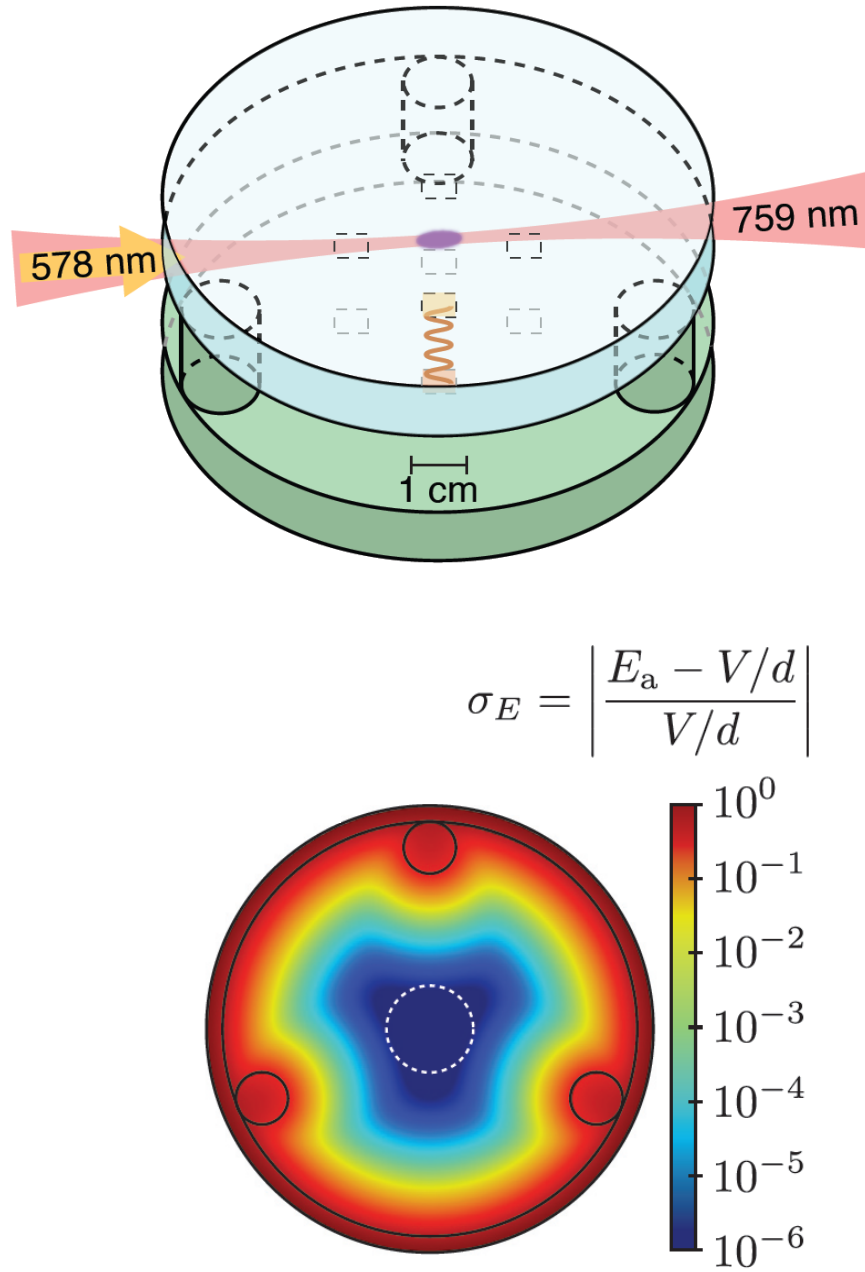


Figure 6.1: Top: Schematic of the electrodes. The lattice and clock light beams thread between the two fused silica plates, which are rigidly spaced by three fused silica spacers as described in the main text. Four pairs of reflective gold pads form planar etalons, which are used to determine the spacer separation. Bottom: Simulation of the electric field produced by the plates. Inside the central 10 mm region (denoted by the dotted white circle), the field deviations are 1 ppm or below. Perturbations due to the three spacers (small black circles) become larger away from the center. The outer black circle denotes the edge of the ITO coating.

## 6.2 Applied electric field

### 6.2.1 Electrode design

To measure  $\alpha_{\text{clock}}$  and reduce the clock's uncertainty due to BBR, we fitted electrodes [226] to the existing ytterbium clock apparatus. The electrodes, shown in Fig. 6.1, are comprised of two parallel fused silica plates (diameter  $D \simeq 102$  mm with better than  $\lambda/10$  flatness) with a transparent conductive coating on the inner surfaces. This conductive layer is made from 0.3 nm of indium-tin-oxide (ITO) [227]. The outer surfaces of the plates are anti-reflection coated for all laser-cooling wavelengths. The electrode separation  $d \approx 15$  mm is maintained by three fused silica rods bonded 45 mm from the center axis with hydroxide catalysis [228, 229].  $d$  is determined interferometrically by *in situ* measurement of the free-spectral-range ( $\nu_{\text{fsr}} = c/2d \approx 10$  GHz) of planar etalons formed by reflective metallic pads. These 90 %-reflectors are 33 nm-thick gold deposited over the ITO layer with a 2 nm chromium adhesion layer in between [226]. Each 6 mm square pad is offset 28 mm from the electrode center.

A voltage  $V_a$  on ideal electrodes spaced by  $d$  in vacuum creates an electric field  $E_a = V_a/d$ , shifting the clock transition by  $\Delta\nu = -\frac{1}{2}\alpha_{\text{clock}}(V_a/d)^2$ . Deviations from this infinite-parallel-plane capacitor model are minimized by designing a large diameter-to-spacing ratio ( $D/d$ ), ensuring a high degree of parallelism, and centering the atoms radially within the electrodes. Numerical modeling reveals that, for our electrodes, these deviations are bounded at the  $10^{-6}$  (1 ppm) level, and perturbations due to dielectric and conducting mounting structure contribute similar amounts of field uncertainty. The lower panel of Fig. 6.1 demonstrates this by plotting the quantity  $\sigma_E \equiv \left| \frac{E_a - V_a/d}{V_a/d} \right|$ , which is a measure of the fractional deviation from the ideal field, as a cross-section of the field distribution. In the central region (10 mm radius, shown by the dotted white circle), the field deviations are at the level of a few ppm. The model also includes errors associated with any small tilt ( $\theta_{\text{wedge}}$ ) between the two plates and the warping of the fused silica plates under the pull of gravity. In the former case, we find that a high degree of parallelism is needed to exclude effects of tilt. For example,  $\theta_{\text{wedge}} \sim 10 \mu\text{rad}$  produces an electric field error of a few ppm. For this

reason, the three fused silica spacers were manufactured to have nearly identical lengths, to within the tolerances for precision glass machining. By measuring the separation  $d$  on each set of planar etalons, we were able to tightly constrain  $\theta_{\text{wedge}}$  and the associated error in  $E_a$  (Sec. 6.2.3).

### 6.2.2 Voltage source and measurement

We constructed a regulated high voltage source as described in [230] that produced up to 1050 V in 100 V increments (Fig. 6.2, top). The circuit utilizes a precision 100:1 divider to compare the high voltage output to a low-voltage reference. A high voltage power MOSFET is used to control the fraction of the unregulated high voltage that is dropped on a resistor in order to achieve a regulated output. With a precision voltmeter, we monitored the regulated high voltage output and found its fractional instability as  $\lesssim 1 \times 10^{-6}$  from 1–1000 s (Fig. 6.2, bottom).

A relay network connects the regulated high voltage to the electrodes through a vacuum feedthrough, and logic signals control the configuration (high voltage or ground) of each plate. Thin strips of silver-loaded epoxy join insulated wires to the electrode perimeters. Two wires were bonded to each electrode to establish the sheet resistance of the conductive layer ( $R_{\text{ITO}} = 3 \text{ k}\Omega$ ). We observed a small leakage current when monitoring the voltage dropped across a large resistor, indicating the parasitic resistance between the electrodes and the grounded vacuum structure is  $R_{\text{leak}} = 316(9) \text{ G}\Omega$  ( $R_{\text{leak}} = 14.3(5) \text{ G}\Omega$ ) below (above) an observed field-emission threshold occurring near  $V_a \approx 800 \text{ V}$ . Leads to the electrodes have current-limiting resistances of  $10 \text{ k}\Omega$  each; at the highest voltages tested, the worst-case error in  $E_a$  from voltage division is 1.4 ppm.

The regulated high voltage was monitored with two commercial voltmeters (both Agilent 3458A, one with Option –002, which includes a higher stability voltage reference) with recent calibrations. According to the manufacturer’s specifications, the measured voltage has several uncertainty contributors, including a 10 ppm (6 ppm with Option –002) reading error and a 2 ppm calibration error for NIST traceability. Unfortunately, there is an additional uncertainty source that scales as  $V_a^2$ , having a value of 12 ppm at  $V_a = 1000 \text{ V}$ . While most d.c. voltmeters have this rising  $V_a^2$ , one type of instrument (Fluke 8508A) does not; however, we were not able to acquire

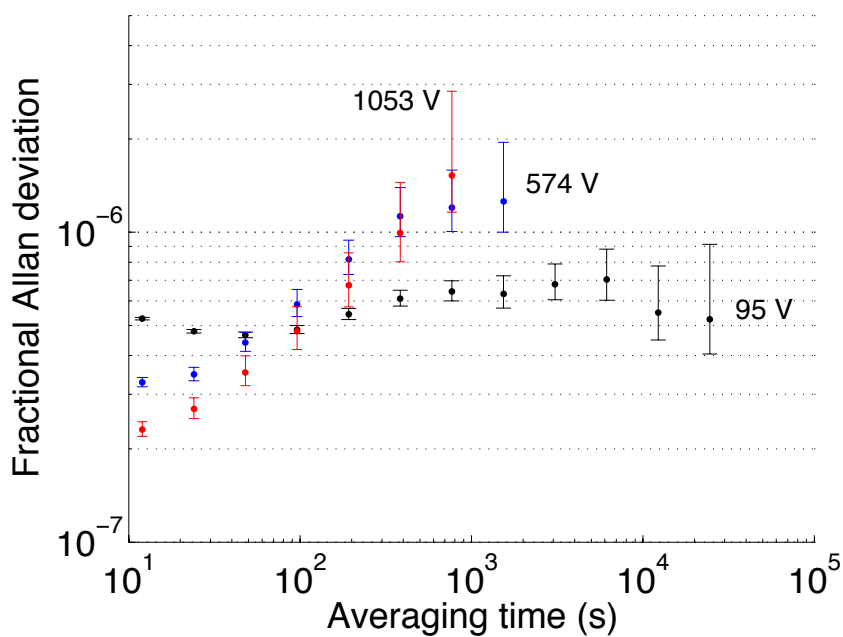
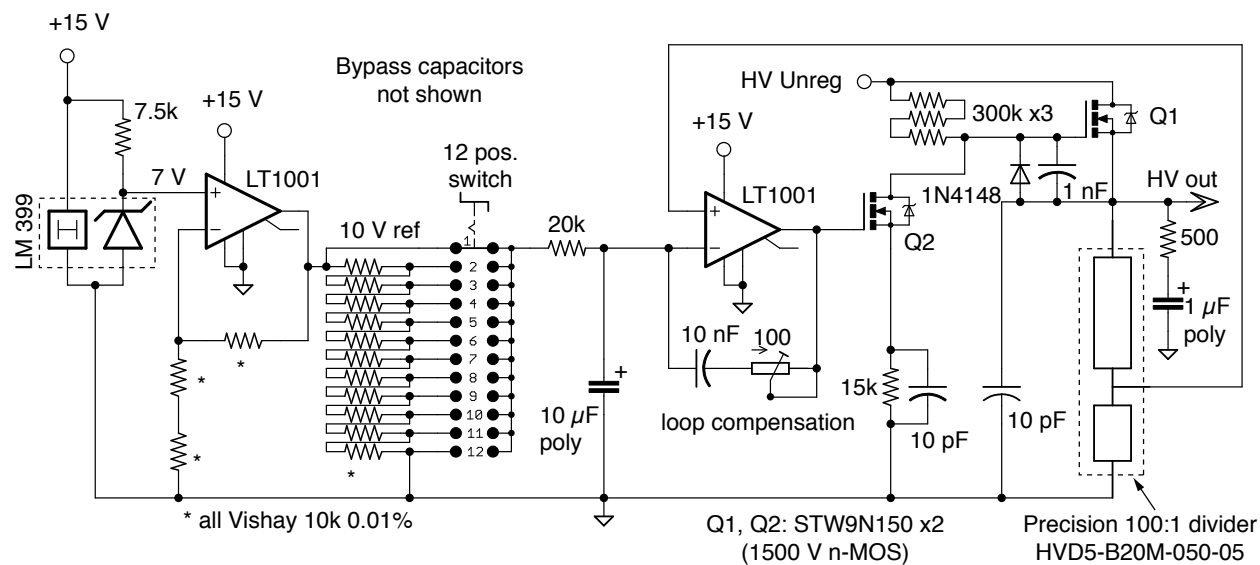


Figure 6.2: Top: Circuit diagram for the regulated high voltage source. A precision 100:1 divider allows for comparing the high voltage output to the low voltage setpoint. Bottom: Allan deviation of the voltage output. The black, blue, and red points correspond to 95 V, 574 V, and 1053 V, respectively.

this instrument in a timely fashion. Note that these uncertainties are given as 95 % confidence; we therefore divided by the stated coverage factor of 1.65 in order to obtain the corresponding 1- $\sigma$  error bar.

The two voltmeters continuously monitored and logged the regulated high voltage. Their readings were found to agree to within a few ppm, much smaller than their specified uncertainties. We took a weighted mean of the two voltage readings in analyzing the final data.

### 6.2.3 Plate separation

The separation between the plates ( $d$ ) was determined by measuring the free spectral range of the etalons formed by the reflective gold pads (Fig. 6.1). An external cavity diode laser was tuned by 17 THz around  $\lambda_p = 766$  nm to observe  $\sim 10$  of the  $N_f \approx 1700$  etalon transmission peaks that fall within the ECDL's tunable bandwidth. Each transmission feature, located with a wavelength meter to  $\pm 50$  MHz, has a linewidth of 500 MHz, consistent with a finesse  $\mathcal{F} \approx 20$ . Spacing the observed peaks logarithmically allows an efficient least-squares determination of  $\nu_{\text{fsr}}$  (Fig. 6.3, top panel) while ensuring the measurement doesn't "slip" a fringe. Round-off error in assigning the mode number to each fringe was typically a few tens of megahertz, much less than the free spectral range ( $\nu_{\text{fsr}} \approx 10$  GHz).

The statistical uncertainty in  $d$ , as determined by the least squares fit, is typically small (1 ppm), due in part to the large number of fringes spanned ( $N_f$ ). Fig. 6.3 (middle panel) shows the error in the least squares determination of  $d$  reduce as more fringes are spanned (moving left to right), and the error is seen to reduce as  $1/N_f$ . However, several systematic effects place the practical limit on knowledge of  $d$ . These include wavemeter and fringe-center-finding inaccuracy, as well as line-pulling from stray etalons (caused, for example, by spurious reflections from the vacuum viewport, the outer surface of the electrode plate, and the electrode-gold interface). In the latter case, we modeled the effects of these stray etalons on the (gold-gold) etalon transmission signal and found line-pulling potentially as large as  $\pm 50$  MHz. Fortunately, the uncertainty in  $d$  due to these systematic effects is also divided down by the number of fringes spanned ( $N_f$ ).

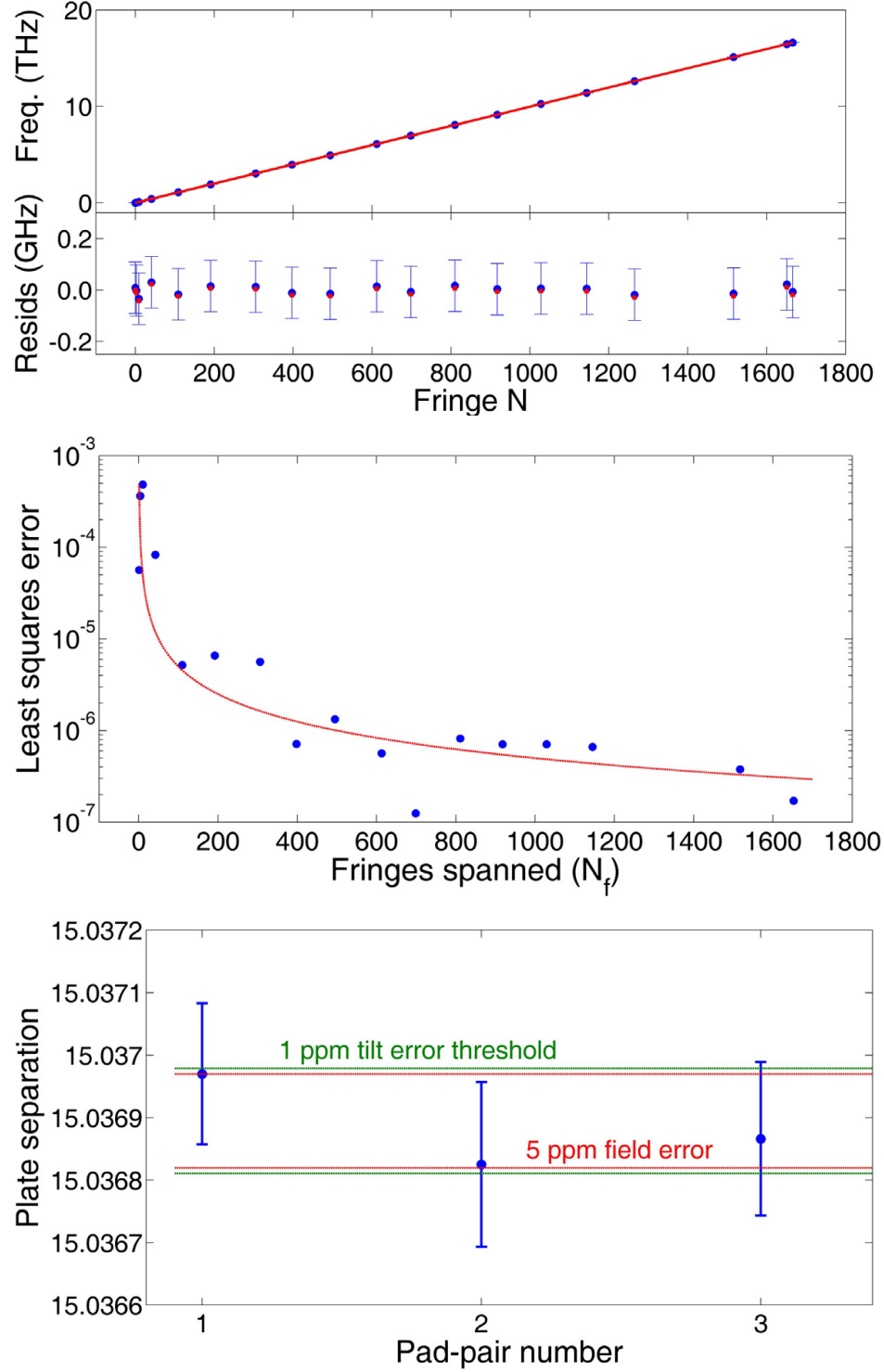


Figure 6.3: Top: The center frequencies of several transmission peaks are monitored. A least squares fit (red line) determines the free spectral range. The residuals (blue) and round-off errors in determining mode numbers (red) are all less than  $\pm 100$  MHz. Middle: The error in the least squares fit (blue points) is shown to decrease as  $\sim 1/N_f$  (red line). Bottom: By measuring  $d$  at several different pairs of gold pads, we constrain the electrode parallelism ( $\theta_{\text{wedge}} \lesssim 4 \mu\text{rad}$ .)



If the laser beam is tilted with respect to the etalon, the apparent free spectral range is slightly increased. The associated fractional error is simply  $1 - \cos(\phi)$ , with  $\phi$  the angle between the probe laser and the cavity axis ( $\phi = 0$  for normal incidence). By ensuring the reflected light was back-coupled into the single-mode fiber that delivered it from the laser, we were able to constrain  $\phi \ll 0.5$  mrad, and the associated uncertainty in  $d$  was below 1 ppm.

Other uncertainty sources include the metal pad thickness (total thickness 33 nm, with uncertainty of a few nanometers) and phase shifts ( $\phi_m$ ) imparted by the gold mirrors. Any change in  $\phi_m$  from one mode to the next causes a small shift to the observed free spectral range:

$$\nu_{\text{fsr}} \equiv \nu_{i+1} - \nu_i = \frac{c}{2d} \left( 1 + \frac{\phi_{i+1} - \phi_i}{2\pi} \right). \quad (6.3)$$

Because  $\phi_m \approx -162.5^\circ$  (calculated using the real index of refraction for gold  $n_r \approx 0.16$  [231]) varies gently about  $\lambda_p$ , variations in  $\nu_{\text{fsr}}$  with fringe index due to mirror phase shifts contribute an error of  $1.2 \times 10^{-6}$ .

Electrode parallelism is constrained by the measured finesse ( $\mathcal{F} \approx 20$ ) as well as spatially independent pad-pair measurements of  $d$ , as in the bottom panel of Fig. 6.3. There, the largest difference (0.0002 mm) between any two pad-pair measurements gives  $\theta_{\text{wedge}} \lesssim 4 \mu\text{rad}$ . Because another data set showed slightly larger disagreement, we take a more conservative value  $\theta_{\text{wedge}} \sim 7 \mu\text{rad}$ , which leads to 2 ppm uncertainty in  $E_a$ .

#### 6.2.4 Stray fields

The cavity-stabilized 578 nm laser was independently locked to the atomic transition under three interleaved conditions: both electrodes grounded (condition ‘A’), and one electrode at high voltage with the other grounded (‘B’ and ‘C’). Each condition, mediated by opto-coupled reed-relays, lasts  $\tau_v = 2.9$  s, during which the clock laser maintains a fractional frequency instability approaching  $3 \times 10^{-16}$ . In each period  $\tau_v$ , four total interrogations are performed: one on each side (e.g. the half-maximum points) of both nuclear-spin spectroscopic features, here driving the usual  $\pi$ -transitions. Slow laser drifts are common to all three integrated error signals  $\Delta\nu_A$ ,  $\Delta\nu_B$ , and

$\Delta\nu_C$  (Fig. 6.4). The quadratic Stark shift is given by

$$\Delta\nu = \frac{1}{2} (\Delta\nu_B + \Delta\nu_C) - \Delta\nu_A. \quad (6.4)$$

Reversing  $\vec{E}_a$  [226] yields information about stray electric fields  $\vec{E}_s$  parallel to  $\vec{E}_a$  or differential contact potentials [232] (e.g. one electrode may develop a thin layer of ytterbium deposition). The quantity

$$\Delta\nu_B - \Delta\nu_C = 2 \alpha_{\text{clock}} \vec{E}_a \cdot \vec{E}_s \quad (6.5)$$

reveals that  $|\vec{E}_s \cdot \hat{z}| \approx 0.1$  V/cm (see Fig. 6.5); temporal drift and weak correlation with  $\vec{E}_a$  are observed. One can easily show that, by taking the average of  $\Delta\nu_B$  and  $\Delta\nu_C$  in Eq. 6.4, the effects of stray fields of any orientation are fully canceled. This assumes, however, that the voltage applied to the two conditions is identical. We tested for the fidelity of the voltage reversal (and hence the stray-field cancelation) and found the fractional difference as  $2(4) \times 10^{-8}$ .

While shifts due to a truly static field  $\vec{E}_s$  subtract completely in Eq. 6.4, time dependent changes, notably those correlated with the polarity of  $\vec{E}_a$ , do not. Because of careful experimental design, we are not aware of any appreciable stray field source with such a correlation. Nevertheless, because an increase in dwell time  $\tau_v$  potentially allows an accumulation of unknown stray charge (and thus a correlated stray field), we varied  $\tau_v$  over 0.8–12 s and resolved a small but negligible correlation in  $\Delta\nu$  at applied fields twice the maximum used for reported data. Under normal operating conditions, the maximal error in  $E_a$  associated with this observed correlation is 1 ppm. We observed no systematic variation in the measured polarizability  $\alpha_{\text{clock}}$  with  $E_a$ , whereas any unknown time-dependent stray charge would likely scale nonlinearly with  $E_a$ . We note that, for data presented here,  $E_a$  remained three orders of magnitude below the dielectric strength<sup>2</sup> of fused silica [233], and five orders of magnitude below the characteristic level [234] for ITO electron emission. The time constant for electrode charging is 8  $\mu$ s; typically, 100 ms is allowed for settling. Connecting high voltage to both electrodes creates an electric-gradient field; by observing  $\Delta\nu < 30$  mHz

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<sup>2</sup> Dielectric strength denotes the maximum electric field an insulator can withstand before breaking down.

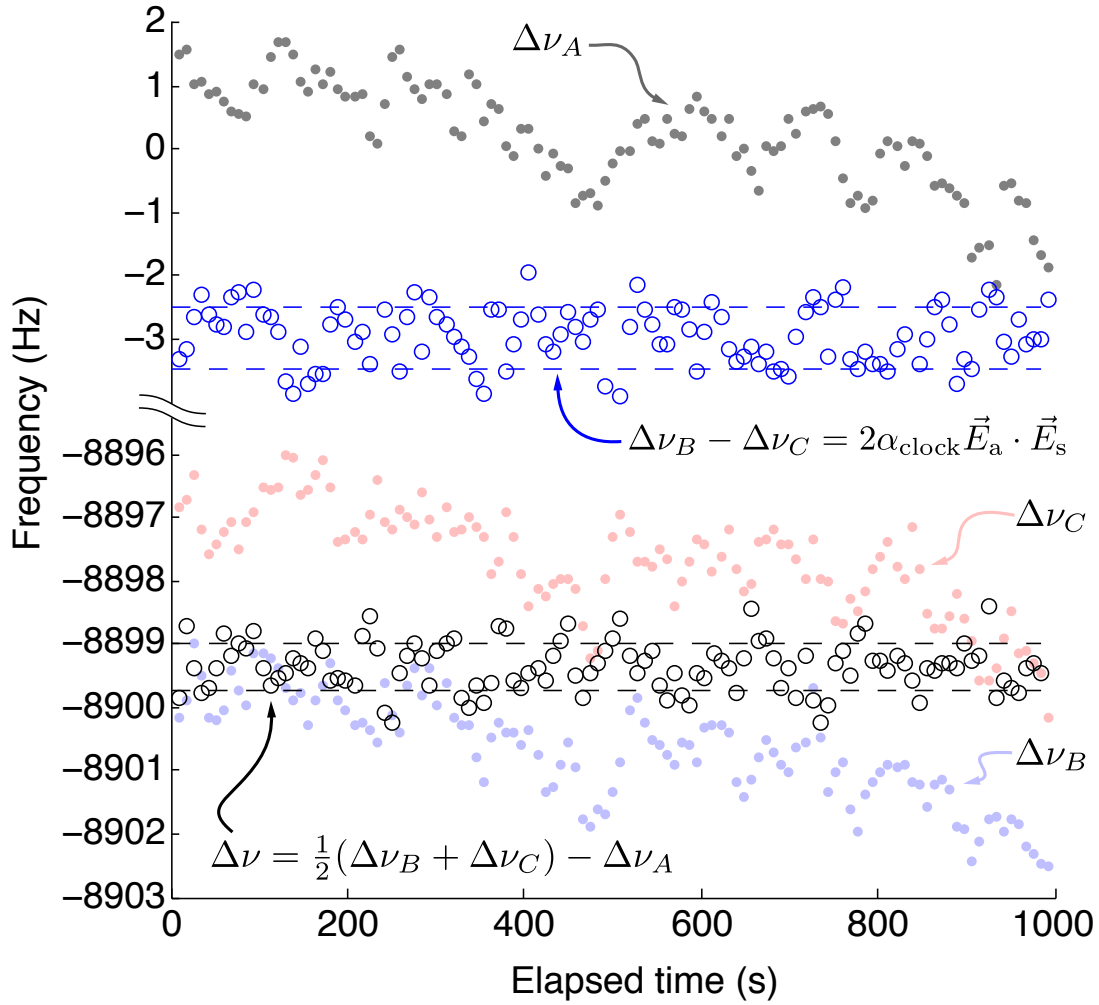


Figure 6.4: A sample data set shows how clock laser drift and stray electric fields are canceled. The clock laser correction signals are shown for  $E_a \approx 700.6$  V/cm under three interleaved conditions: both electrodes ground ('A', grey dots), and one electrode at high voltage with the other ground ('B' and 'C', blue and red dots). The quadratic Stark shift (black open circles) and stray field signal (open blue dots) are shown to be independent of laser drift. Dashed lines show standard deviations for these signals.

with 2 kV applied, we constrain the atoms radial position to  $\pm 10$  mm, consistent with visual observations.

### 6.3 Measurement results

Fig. 6.5(a) shows that the observed clock frequency shifts quadratically as a function of  $E_a$ . When fit to a polynomial using a total least squares algorithm,<sup>3</sup> the data are consistent with no quartic, cubic, linear, or offset terms – an ideal demonstration of the Stark effect as non-degenerate perturbation theory. No inhomogeneous line broadening is observed with increased shift, so the fractional statistical uncertainty in  $\Delta\nu$  reduces as  $E_a^{-2}$ . In contrast, the uncertainty of the applied voltage (the dominant systematic uncertainty) rises as  $E_a^2$  according to the specifications of our commercial voltmeters. Table 6.1 lists the sources of measurement uncertainty at a particular applied field. Fig. 6.5(c) plots the polarizability inferred at each  $E_a$ , and a weighted mean to determine  $\alpha_{\text{clock}}$  agrees well with the value obtained using the least squares algorithm as in part a) of the figure. Taking the mean of all measurements, weighted by the total standard errors, we determine  $\alpha_{\text{clock}} = 36.2612(7)$  kHz/(kV/cm)<sup>2</sup>. Table 6.2 demonstrates the agreement between this measurement and theoretical predictions.

Neither static nor BBR fields cause spin-magnitude-dependent ( $\propto |m_F|^2$ ) tensor Stark shifts because both clock states have insufficient total angular momentum [137] (Sec. 2.3). Spin-sign-dependent ( $\propto m_F$ ) vector Stark shifts are absent as well: BBR has no net polarization, and static fields lack the time dependence to be circularly polarized [235]. No opposite-parity states lie close to either clock state, so no linear dependence of  $\Delta\nu$  on  $E_a$  is expected or observed. A third-order effect [187] mixing the polarization due to the optical lattice ( $E_{\text{lattice}} \approx 10$  kV/cm) with  $E_a$  is expected to cause a  $10^{-9}$  fractional error at the highest  $E_a$ . A fourth-order term  $\Delta\nu \propto E_a^4$  (the d.c. hyper-polarizability) is responsible for a similarly sized effect.

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<sup>3</sup> Total least squares accounts for error bars in both the dependent and the independent variables.

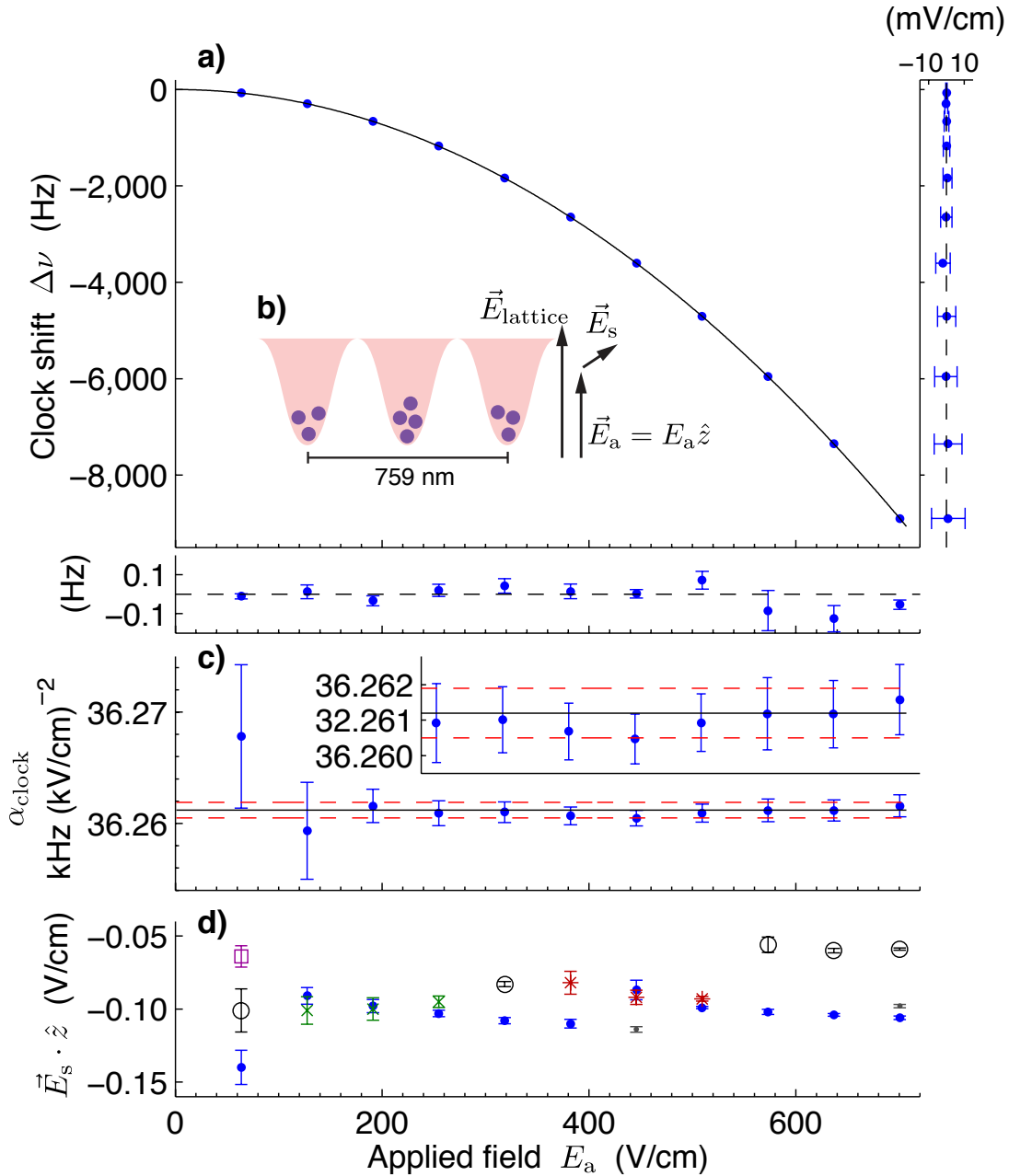


Figure 6.5: Measurement results. a) The frequency shift is observed to be quadratic with  $E_a$ . Residuals of a quadratic effect display measurement uncertainties in  $\Delta\nu$  (below) and  $E_a$  (right). b) An inset depicts lattice trapped atoms and relative orientations of  $\vec{E}_{\text{Lattice}}$ ,  $\vec{E}_a$ , and a hypothetical stray field  $\vec{E}_s$ . c) At each  $E_a$ , we display  $\alpha_{\text{clock}} = -2\Delta\nu/E_a^2$  with combined statistic and systematic uncertainties. An inset shows data at higher resolution. Solid and dashed lines show the final result and standard error, respectively. d) The component of a stray field  $\vec{E}_s \parallel \vec{E}_a$  is precisely detected by reversing  $E_a$ . We observe more temporal variation in  $E_s$  than correlation with  $E_a$ . Data with different marker styles were acquired on separate days.

Table 6.1: Uncertainty budget for a representative datum. Errors in  $E_a$  contribute twice the uncertainty as those in  $\Delta\nu$  due to the dependence  $\alpha_{\text{clock}} = -2\Delta\nu/E_a^2$ . This factor of two is included in the tabulated quantities below. The total uncertainty in  $\alpha_{\text{clock}}$ , for the particular measurement shown, is found by summing all contributions in quadrature.

| Uncertainty source                     | $\times 10^{-6}$ | Notes/conditions                                               |
|----------------------------------------|------------------|----------------------------------------------------------------|
| Shift statistical error                | 8.3              | $\Delta\nu = -3603.77(3)$ Hz (1800 s averaging)                |
| Voltage ( $V_a$ ) errors:              |                  | regulated 670.397(6) V                                         |
| voltmeter systematic                   | 16.4             | weighted mean of two voltmeters                                |
| $R_{\text{leak}}$ voltage division     | 0.1              | $I_{\text{leak}} = 2.1$ nA; 20 k $\Omega$ leads                |
| Separation ( $d$ ) errors:             |                  | $d = 15.03686(8)$ mm                                           |
| statistical                            | 1.6              | $N_f > 1700$ fringes spanned                                   |
| systematic                             | 9                | fringe centering, wavemeter accuracy, stray etalons, stability |
| etalon probe tilt, $\phi$              | 0.3              | $\phi \ll 0.5$ mrad by retro-coupling to single-mode fiber     |
| Other field ( $E_a$ ) errors           |                  | $E_a = 445.836(4)$ V/cm                                        |
| stray fields, static                   | 0.08             | uncertainty in $\vec{E}_a$ reversal                            |
| stray fields, varying                  | 2                | $\Delta\nu$ correlation with $\tau_v$                          |
| finite electrode size                  | 1                | atoms centered $\pm 10$ mm                                     |
| dielectric spacers                     | 2                | perturbation due to three fused silica posts                   |
| electrode parallelism                  | 4                | $\theta_{\text{wedge}} < 7$ $\mu\text{rad}$                    |
| electrode deformation                  | 0.8              | warping of fused silica by gravity                             |
| Yb thermal beam                        | 0.06             | dielectric constant $(\epsilon_r - 1) \sim 8 \times 10^{-9}$   |
| Higher-order Stark shifts              | 0.01             |                                                                |
| Uncertainty in $\alpha_{\text{clock}}$ | 21               |                                                                |

Table 6.2: Comparison with theoretical predictions. Results are also presented in SI and frequently used atomic units (a.u.) [124].

$$\alpha_{\text{clock}} \equiv \alpha_e^{(0)} - \alpha_g^{(0)}$$

| [ kHz (kV/cm) <sup>-2</sup> ] | [ a.u. ]   | 10 <sup>-39</sup> [C m <sup>2</sup> /V] | Reference |
|-------------------------------|------------|-----------------------------------------|-----------|
| 40.1(3.7)                     | 161(15)    | 2.65(25)                                | [194]     |
| 38.6(4.0)                     | 155(16)    | 2.56(26)                                | [221]     |
| 33(13)                        | 134(51)    | 2.21(84)                                | [236]     |
| 36.2612(7)                    | 145.726(3) | 2.40269(5)                              | this work |

For presented data,  $\vec{E}_a \parallel \vec{E}_{\text{lattice}}$ , and both were perpendicular to the magnetic field  $\vec{B}$ , though other configurations were examined. We observed no change in  $\Delta\nu$  upon varying the lattice intensity or polarization. We ensured that the atomic density did not systematically vary with application of  $E_a$ ; such a correlation could introduce contamination from the cold collision shift [213]. We resolved no shift by systematically varying the electrodes between grounded and floating configurations. Finally, we observed no variation in Zeeman splitting with application of  $E_a$ .

We note that our present uncertainty in  $\alpha_{\text{clock}}$  is competitive with the best known atomic or molecular polarizability, that of helium [237]. Beyond timekeeping, possible metrological applications of the present work include high voltage measurement without the use of resistive dividers or an atomic electric field meter sensitive at moderate field strengths, in contrast to Rydberg atoms [238], which are most sensitive at very low fields.

## 6.4 Controlling the BBR shift at 10<sup>-18</sup>

Having accurately determined the differential polarizability of the Yb clock transition, we can now reassess the implications for the BBR shift and its uncertainty. There are three potential sources of error that we must consider.

i) First, an inaccurate determination of the atomic sensitivity to blackbody radiation will cause an error in the extrapolation back to the BBR-free temperature of absolute zero. The atomic response is almost entirely summarized by the static polarizability,  $\alpha_{\text{clock}}$ , which was measured at

the 20 ppm level, supporting a BBR uncertainty below  $10^{-19}$ . But, as noted above (Eq. 6.2), true BBR fields are not static but are instead centered in the mid-infrared ( $9.6 \mu\text{m}$  for 300 K). We can account for the enhancement of BBR effects due to near-resonant couplings with the parameter  $\eta_{\text{clock}}$  as in Eq. 6.1. The dynamic correction for state  $|i\rangle$  ( $i = \{e, g\}$ ) can be found by summing over all intermediate states  $|k\rangle$  as in [221] (here in atomic units):

$$\eta_i = \frac{80 \pi^2}{63 \alpha_i^{(0)} T} \sum_k \frac{|\langle k | \hat{d} | i \rangle|^2}{2 J_i + 1} \left( 1 + \frac{21 \pi^2 T^2}{5 \omega_k^2} + \frac{336 \pi^4 T^4}{11 \omega_k^4} \right) \quad (6.6)$$

with  $\hat{d}$  the electric dipole operator,  $\omega_k$  the transition frequency between states  $|i\rangle$  and  $|k\rangle$ , and  $T$  the temperature. For Yb, the dominant contribution to this dynamic polarizability comes from the  $^3P_0 \leftrightarrow ^3D_1$  transition near 1388 nm; the next largest contributors are the  $^3P_0 \leftrightarrow ^3S_1$  transition near 649 nm and the  $^1S_0 \leftrightarrow ^1P_1$  transition near 399 nm, both of which produce effects more than ten times smaller.

Thus, the value of the  $^3P_0 \leftrightarrow ^3D_1$  reduced matrix element is critical for accurately determining  $\eta_{\text{clock}}$ , but experimental and theoretical efforts to determine this value disagree. The relativistic many-body calculation of *Dzuba and Derevianko* [194] gives this value as  $2.91 a_0$  ( $a_0$  the Bohr radius), while the lifetime measurement of *Bowers, et al* [121] gives the value as  $2.60 a_0$ , provided one assumes the branching ratios follow *LS*-coupling, which those authors suggest is a valid assumption. The two curves of Fig. 6.6 show the calculated  $\eta_{\text{clock}}$  as a function of temperature using the two values for the  $^3D_1$  matrix element given above, along with all other states listed in Table 2.1. As shown in the figure, at room temperature ( $T_r = 300 \text{ K}$ ), we find  $\eta_{\text{clock}}(T_r) = 0.0156$  using the experimental value, and  $\eta_{\text{clock}}(T_r) = 0.0196$  using the theoretical value. From these, we take the mean  $\eta_{\text{clock}}(T_r) = 0.0176(20)$ . This uncertainty corresponds to 2 parts-per-thousand of the total BBR shift, or about  $5 \times 10^{-18}$  fractional frequency. So, inside an ideal blackbody at exactly 300 K, the Yb clock frequency is reduced from its value at 0 K by  $2.465(5) \times 10^{-15}$ .

Future efforts to constrain the  $^3D_1$  matrix element (which, if determined by a lifetime measurement, also requires knowledge of the branching ratio) will directly reduce this uncertainty, perhaps to the level of  $1 \times 10^{-18}$ . Alternatively, the clock could be operated in a cryogenic envi-



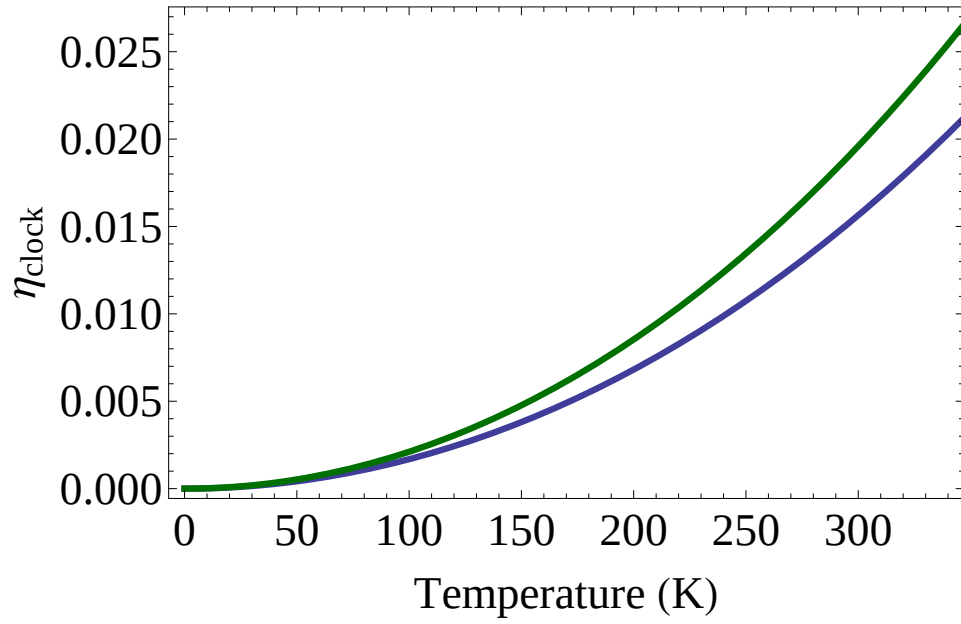


Figure 6.6: Shown is a calculation of  $\eta_{\text{clock}}$  using the states listed in Table 2.1 as a function of temperature. The two lines differ in their choice of matrix element for the lowest-lying transition,  $(6s6p) {}^3P_0 \leftrightarrow (5d6s) {}^3D_1$  at 1388 nm. The blue curve uses  $2.42 a_0$  as in [121] while the green curve uses  $2.91 a_0$  as in [194] ( $a_0$  the Bohr radius).

ronment as discussed below; at liquid nitrogen temperature of 77 K,  $\eta_{\text{clock}} = 0.0011(2)$ . At that temperature, the Yb clock frequency is shifted by  $1.07 \times 10^{-17}$ , and the uncertainties in  $\eta_{\text{clock}}$  and  $\alpha_{\text{clock}}$  are both negligible.

ii) A second source of error from the BBR shift arises from an inaccurate measurement of the temperature of the pseudo-blackbody surrounding lattice-trapped atoms. With standard techniques, it should be possible to measure and control the temperature of an all-metal vacuum chamber with less than 1 K of uncertainty. Unfortunately, at room temperature, the slope of the BBR shift is somewhat steep ( $3.3 \times 10^{-17}/\text{K}$ ), leading to a non-negligible clock uncertainty. While it may be possible to make temperature measurements at or below the 100 mK uncertainty level, it instead could be easier to reduce this uncertainty contribution by cooling the apparatus, benefitting from the  $T^3$  scaling of the slope of the BBR vs. T curve. At 77 K, the sensitivity to temperature is  $5.6 \times 10^{-19}/\text{K}$ , indicating a 1 K temperature uncertainty would suffice.

iii) The third source of error is the BBR shift associated with radiation that deviates from that of an ideal blackbody. For example, in our current Yb experiment, there are numerous glass viewports in the vacuum chamber, and these are not necessarily at the same temperature as the stainless steel chamber, nor are they perfectly opaque to radiation originating elsewhere in the laboratory. Similarly, the extremely hot oven, nozzle, and heated window all have a direct line-of-sight to the atoms, though with limited solid angle; moreover, the interior of the vacuum chamber is presumably not a perfect blackbody absorber (i.e. the emissivity deviates from unity), so that this radiation could take multiple reflections off the chamber walls (and have multiple chances to polarize the atoms) before being absorbed. Effects such as these, though likely small effects in comparison to the relatively large ( $10^{-15}$  level) total BBR shift, will likely place the practical limit on how well the BBR shift can be controlled in lattice clocks. Importantly, this source of uncertainty cannot be reduced with cryogenic operation.

To overcome item iii), many groups have considered housing the lattice-confined atoms inside a specially-designed thermal shield [225, 1], which typically would fit inside a more standard vacuum

chamber. The thermal environment would be designed to have limited optical access and high emissivity. In addition to minimizing the total number and size of any openings, it is critical to move these openings far away from the atoms to decrease the solid angle through which radiation can directly penetrate. Moreover, a high emissivity ensures that any leak-through radiation that does not follow the line of sight gets quickly absorbed. Finally, many groups are also considering the option of cryogenically cooling this thermal shield, which would largely remove uncertainty terms i) and ii) above.

Presently lacking this type of well-defined thermal environment, we place a 1 K uncertainty on the blackbody environment, and, for the time being, the BBR uncertainty is  $\sim 3 \times 10^{-17}$ . Just how well the BBR shift can truly be controlled in future lattice clocks is still an open and important question.

## Chapter 7

### Clock Comparisons and Evaluations

Each of the previous three chapters treated a physical effect (lattice light shifts, atom-atom collisions, and Stark shifts from blackbody radiation) that is relevant to optical lattice clocks. In those studies, we used the superb frequency resolution of the clock to learn about the physical phenomena in a highly-controlled manner. Of course, the motivation for these studies was not just to learn the physics, but also to measure and (ideally) reduce the systematic effects that contribute to the clock error budget. Not coincidentally, those three effects are the most relevant systematic effects for high-performance lattice clocks.

For some of the applications given in Sec. 1.3, including precise tests of relativity, constraints on the time-dependence of fundamental constants, and the realization of the SI second, the clock's total systematic uncertainty<sup>1</sup> is a critical parameter. To date, the best characterized clock of any kind claims a total systematic uncertainty of  $8.6 \times 10^{-18}$  [37], while the best characterized lattice clock claims a total systematic uncertainty of  $1.5 \times 10^{-16}$ . In this section, we will examine all known systematic effects that could lead to clock errors and determined what number should be assigned to the  $^{171}\text{Yb}$  lattice clock.

#### 7.1 Systematic evaluation of $^{171}\text{Yb}$ lattice clock

To evaluate systematic shifts of the clock frequency, we performed a series of optical comparisons against the Ca optical standard at NIST [239] with a self-referenced femtosecond-laser

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<sup>1</sup> Some metrologists use “total systematic uncertainty” interchangeably with “accuracy,” but in fact no clock can accurately realize the SI second except for cesium.

frequency comb [240, 241]. The Ca clock was configured to run in a higher-stability mode, bypassing a second stage of laser-cooling in favor of a shorter cycle time and reduced Dick effect [242]. During these measurements, the fractional frequency instability between the two clocks started at  $5 \times 10^{-15}$  at 1 s and averaged down to  $3 \times 10^{-16}$  at 200 s. On longer time scales, drifts in the Ca clock degrade the stability, so typically data sets were taken in repeated bins of 200 s. To partially cancel the Ca drift, we alternated between two conditions of a particular systematic effect in an antisymmetric pattern. For example, to measure the collision shift, we alternated between high atomic density ('A') and low atomic density ('B') using the pattern A-B-B-A. This was repeated many times to gain confidence in the result and reduce statistical error.

The frequency comb was typically configured as shown in Fig. 7.1. The comb's repetition rate was stabilized (via an intra-cavity PZT) to the Ca clock, while the comb's offset frequency was self-referenced using an  $f - 2f$  interferometer [241], with appropriate feedback to the laser pump power. With these two feedback mechanisms, the stability of the Ca clock is transferred throughout the comb spectrum, allowing for comparisons between the Yb and Ca clocks. One difficulty in using a Ti:sapphire frequency comb is producing sufficient optical power near 578 nm to generate a high signal-to-noise beat signal with the Yb laser. Fortunately, with special microstructured fibers [243], this wavelength can be reached with (just enough) optical power to make the measurements. This beat signal between Yb and one comb tooth was monitored with an electronic counter (Agilent 53132A, 1 s gate time) whose output was transferred to a computer via GPIB.

The Ca clock, conveniently co-located in our laboratory, proved to be an excellent tool for making the first evaluation of the Yb lattice clocks (both  $^{174}\text{Yb}$  and  $^{171}\text{Yb}$ ). The initial observations of density-dependent collision shifts (Sec. 5.1) and magic wavelength measurements (Sec. 4.1) relied on these optical frequency comparisons with the Ca clock. Below, we discuss several other important systematic effects that were also measured in this manner, leading to a reported total systematic uncertainty of  $3.4 \times 10^{-16}$  in 2009. However, the lack of long-term stability in the Ca clock makes it difficult to reasonably claim statistical uncertainties below  $10^{-16}$ . Moreover, as the lattice clock was pushed to higher stability, thanks largely to improvement in the optical cavities (Sec. 3.5), it

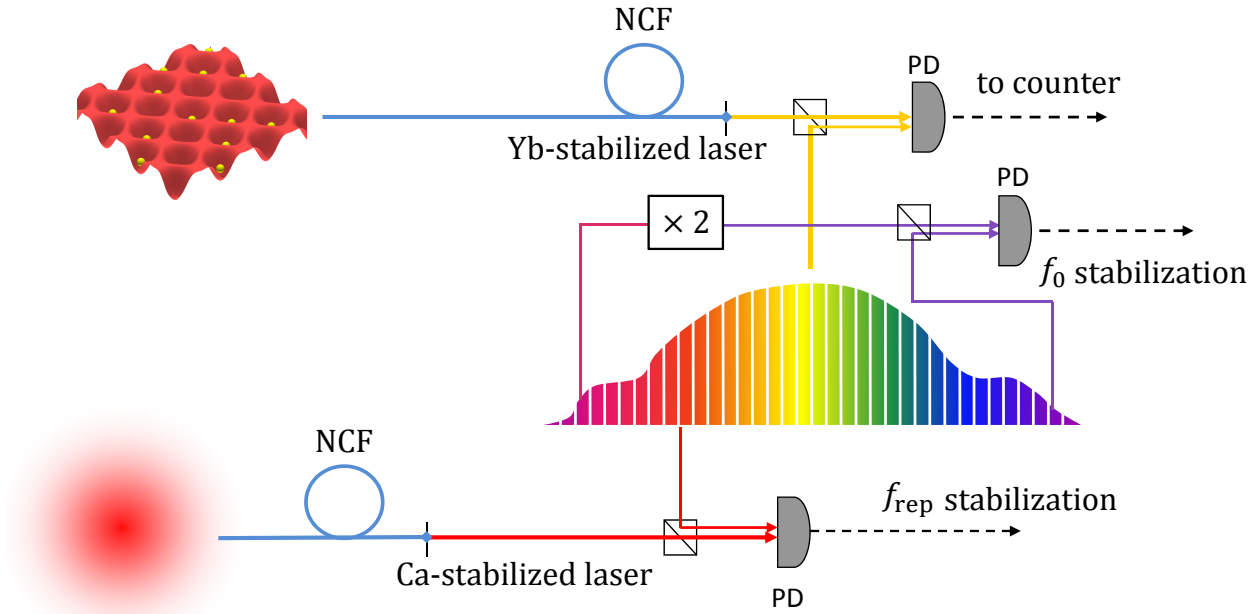


Figure 7.1: Setup for measuring systematic effects relative to the Ca clock with a frequency comb. Laser light near 657 nm, referenced to the Ca optical clock transition, is carried by noise-canceled fiber (NCF) to an adjacent laboratory that contains the octave-spanning frequency comb [241]. The comb's repetition rate ( $f_{\text{rep}} \simeq 1$  GHz) is locked to the Ca-stabilized laser, with feedback to a piezo-electric transducer inside the comb's laser cavity. Because the offset frequency ( $f_0$ ) has also been locked via the  $f - 2f$  interferometer [241], the Ca stability is transferred throughout the entire comb spectrum. Near 578 nm, a beat frequency between one comb tooth and the Yb-stabilized laser (also delivered by noise-canceled fiber) is counted with an Agilent 53132A (1 s gate time), and the counted frequencies are monitored and binned to determine the measurement results.

became less appealing to average through the Ca short-term noise when a higher-stability option was available. For these reasons, in 2010 we began making systematic measurements relative to the optical cavity, as described in Sec. 3.6, a technique which recently was used for analyzing collision effects (Ch. 5) and static polarizability (Ch. 6). These results comprise the first part of a re-evaluation of the  $^{171}\text{Yb}$  lattice clock that, hopefully, will be complete by the end of 2012. The following discussion also includes the prospects for reducing the 2009 uncertainties as part of the 2012 evaluation, though it should be noted that this evaluation remains a work in progress.

### 7.1.1 Zeeman shifts

As discussed in Sec. 2.3, one of the main effects of nuclear spin is to introduce (via the hyperfine interaction) first-order Zeeman sensitivity. The splitting of each  $\pi$ -transition (from line center) is around 200 Hz/G. We typically apply a magnetic field just over 1 G, producing a  $\pm 250$  Hz shift. Averaging over both  $\pi$ -transitions, which is accomplished with a suitable feedback loop to the “chopping” AOM between the 578 nm laser and the atoms (AOM3 in Fig. 3.7), should fully cancel this shift. However, the second-order Zeeman shift ( $\Delta\nu = \beta B^2$ ) is common to both  $\pi$ -transitions and is not canceled by averaging. The second-order shift can be shown to arise from magnetically-induced state mixing, primarily between the  $^3P_0$  and  $^3P_1$  states [185]. For Yb,  $\beta \approx -0.06$  Hz/G<sup>2</sup>, so a  $\sim 1$  G field produces a small shift, of order  $10^{-16}$ .

We measured both Zeeman effects simultaneously by varying the applied field and looking for a clock shift, relative to the Ca clock. The correction signal to the chopping AOM provides a real-time monitor of the magnetic field value, which is found to be proportional to a monitor of the electrical current that creates the bias magnetic field. The clock frequency was measured at three magnetic field values, as shown in Fig. 7.2. Simultaneous linear and quadratic fits reveal coefficients  $+20(19)$  mHz/G and  $-0.072(5)$  Hz/G<sup>2</sup>, respectively. As expected, the first-order effect is well-canceled, while the second-order effect is clearly resolved and consistent with theoretical predictions [185] and previous measurements [90].

With the narrower ( $\sim 1$ – $2$  Hz) spectral features afforded by improvements to the clock laser,

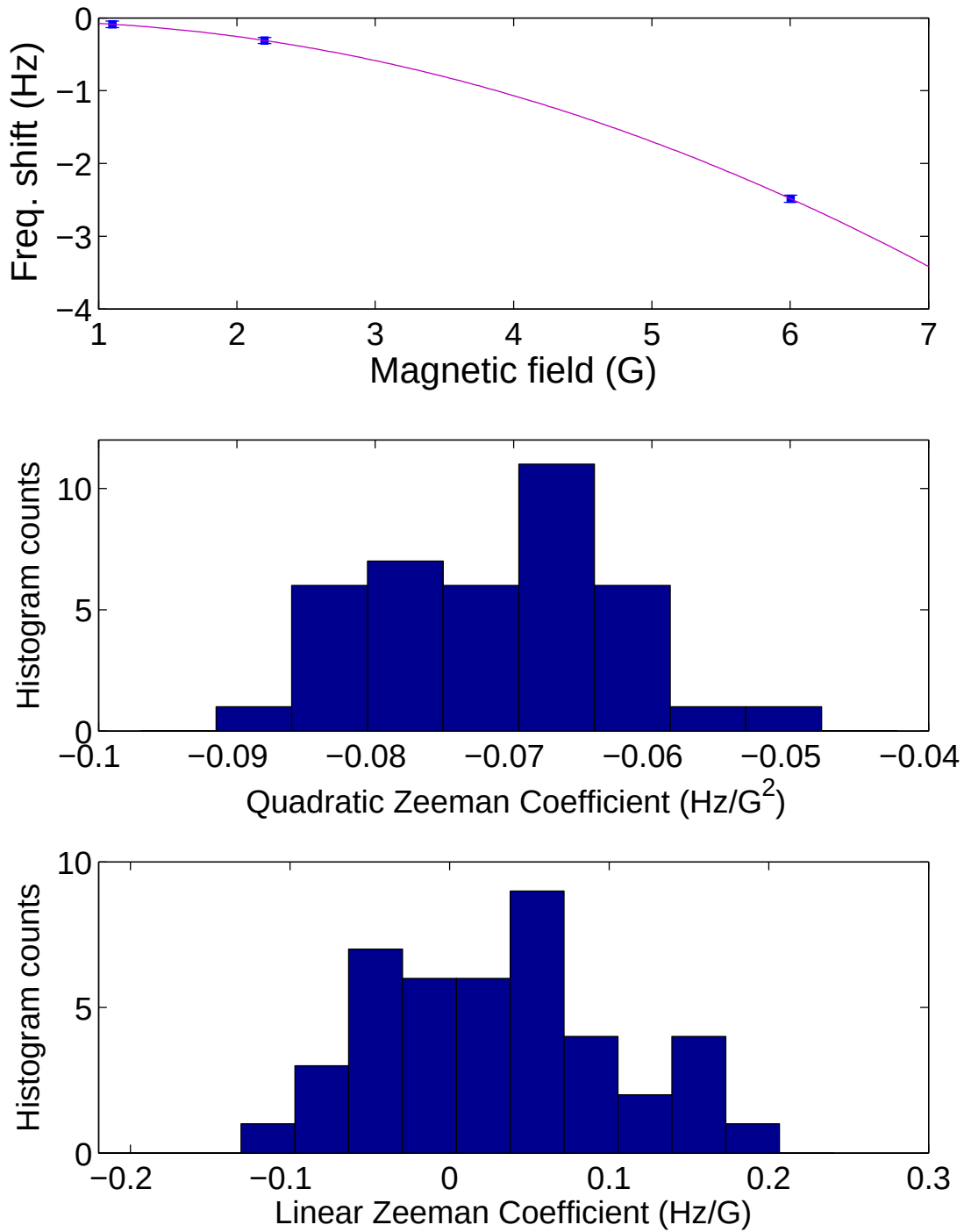


Figure 7.2: Top: clock frequency versus magnetic field strength. Middle: histogram of 2nd-order Zeeman coefficient. The weighted mean is  $-0.072(5)$  Hz/G<sup>2</sup>, where the uncertainty comes mainly from calibrating the magnetic field. Bottom: histogram of 1st-order Zeeman coefficient. The mean is  $+20(19)$  mHz/G, mostly consistent with zero.



it may be convenient to reduce the size of the magnetic field, since the various Zeeman components are quite cleanly resolved. For example, reducing the field by a factor of five would reduce the second-order Zeeman shift to below  $10^{-17}$ , while the two  $\pi$ -transitions would be still be easily resolved, split by  $\pm 50$  Hz. In this case, the uncertainties associated with the Zeeman effects are both well below  $10^{-17}$ , and with further measurements to reduce statistical errors, an additional factor of ten reduction should be straightforward.

### 7.1.2 Probe light shift

In addition to resonantly driving the clock transition, the 578 nm clock probe light causes a Stark shift due to off-resonant couplings between one clock state and another intermediate state [185, 224]. The dominant contributions are the  $^1S_0 \leftrightarrow ^1P_1$  and  $^3P_0 \leftrightarrow ^3S_1$  transitions near 399 nm and 649 nm, respectively. The dynamic polarizability at 578 nm can be calculated using Eq. 2.15 and the states listed in Table 2.1, which yields a shift coefficient of 17 mHz/(mW/cm<sup>2</sup>). In  $^{174}\text{Yb}$ , where a much higher intensity is needed to efficiently drive the clock transition [185, 90], the probe light shift coefficient was measured to be 15(3) mHz/(mW/cm<sup>2</sup>), which agrees well with the calculation.

For Rabi spectroscopy of  $^{171}\text{Yb}$ , we measured that a probe light intensity  $I_p \approx 0.2$  mW/cm<sup>2</sup> produces a  $\pi$ -pulse in 80 ms. Intensities this low produce a Stark shift of only a few mHz – mostly negligible for our first evaluation [43].

However, with Ramsey spectroscopy, the short pulses require higher intensity and produce larger shifts, even accounting for the fact that the total shift is diluted by the dark time (when there is no shift). For any shift that is present only during the Ramsey pulses, the net shift can be written [244]

$$\Delta\nu = \frac{\Delta\nu_p}{1 + (\pi/4)(T/\tau)} \quad (7.1)$$

with  $\Delta\nu_p$  the shift during the pulses,  $T$  the dark time, and  $\tau$  the pulse time. With the Ramsey scheme used to demonstrate cancelation of the the collision shift in Sec. 5.6 (10 ms pulses and

150 ms dark time), the probe light shift is  $+5(3)$  mHz.

### 7.1.3 AOM phase chirp

Between the 578 nm laser and the atoms, the clock light passes through a “chopping” AOM. The purposes of this AOM are three-fold: first, it is used for shuttering the light on and off; second, the AOM frequency is dithered on each side of the spectroscopic line to create an error signal; and third, it is used to lock onto the Zeeman splitting between the two nuclear-spin spectral features, as discussed above. Because this AOM is not seen by the frequency comb, it is essential that the RF that drives the AOM be well-characterized; for that reason, the synthesizer time-base is derived from the NIST timescale.

AOMs are remarkable devices, in that they (almost) perfectly add the RF frequency to the optical frequency with no error. However, any small phase chirp produced by the AOM could lead to a frequency shift. A previous test with a Ca clock [245] revealed two distinct phase chirp effects: one a “ringing” effect associated with the first surge of RF entering the device, and the second a heating effect. The ringing effect is relevant on the timescale of micro-seconds; even for the large ( $\sim 10^{-13}$ ) effects reported, it should be minuscule when averaged over an 80 ms (or longer) spectroscopic time. However, the heating effect was observed at longer timescales and needs careful consideration here.

We tested for phase chirps by employing a heterodyne Michelson interferometer, wherein one arm passed through the AOM, and the other did not (both were then retro-reflected, recombined, and photodetected). This produces a beat signal at twice the AOM frequency ( $2 \times 200$  MHz). This tone was amplified, bandpass filtered, mixed to d.c. by subtracting out twice the AOM’s RF signal, low-pass filtered ( $\sim 30$  kHz), and monitored on an oscilloscope. One important step was to add a tunable phase delay to one arm of the RF to ensure the interferometer was operated near the point of highest sensitivity; this was adjusted while shaking the optical table to produce a maximal signal.

The measurement results are shown in Fig. 7.3. In the top panel, a sample data set is

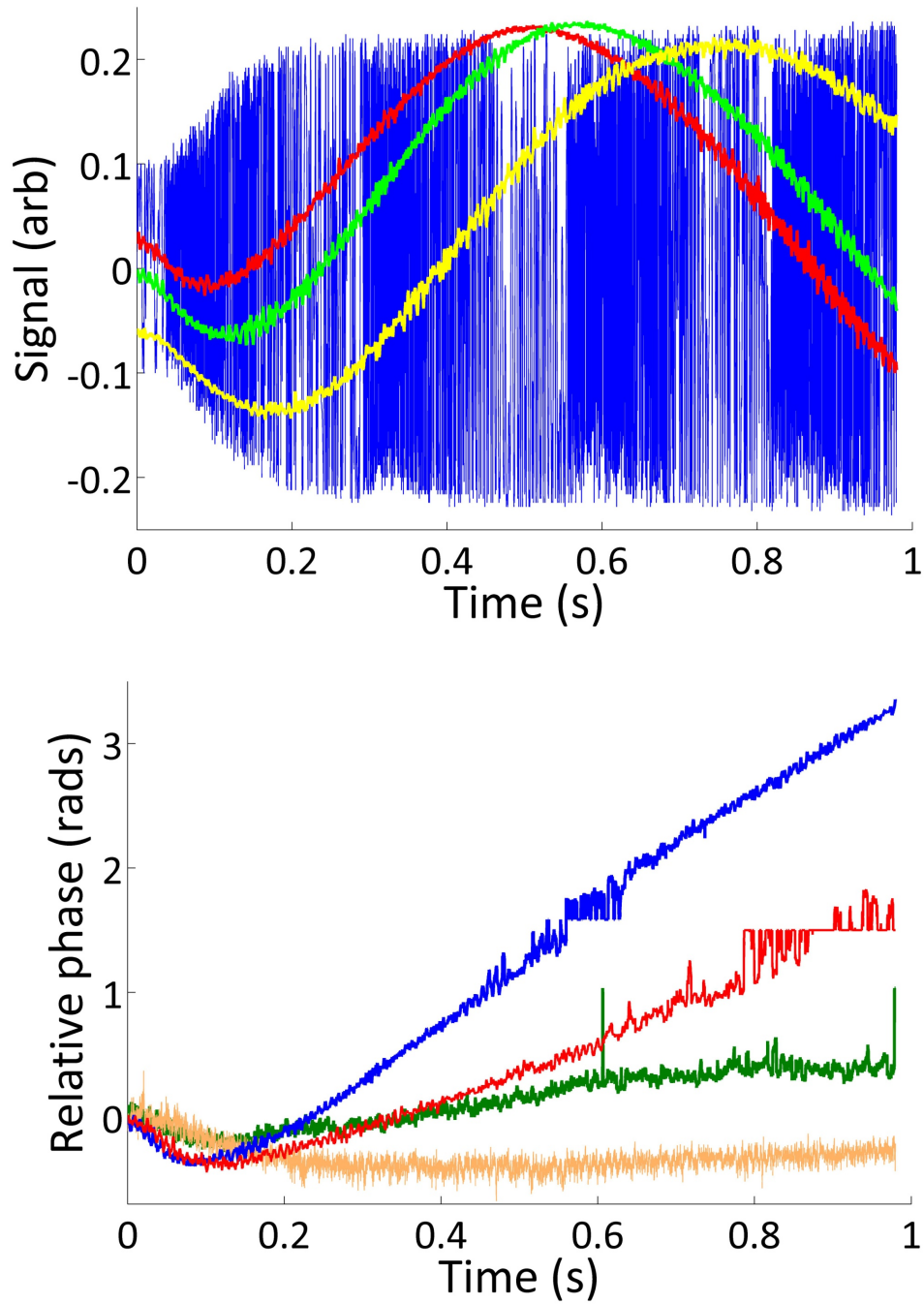


Figure 7.3: Top: Typical raw data from the AOM phase chirp measurement. The blue lines correspond to when we shook the table to determine the full range of the interferometer. The three colored lines show the phase excursion in three separate instances. Bottom: determined phase excursion over time. The four colors correspond to four different RF power levels, with blue the highest (nominally full power), and red/green/orange each 2–3 dB lower than the previous.

shown. The blue signal was recorded as we shook the optical table by hand, thus wrapping the phase of the interferometer very quickly to observe its limits. The red, green, and yellow curves are three successive data sets, with the AOM set to maximal power. After about 100 ms, the heating-induced phase chirp changes sign, presumably due to differing time constants associated with heating different aspects of the device. In the lower panel, we extract the phase excursion for four different RF powers. The blue curve correspond to the highest RF power as in the top panel, while the red, green, and orange curves are each 2-3 dB lower than the previous. At maximal RF power, the phase chirp is 4.7 rad/s, which equates to a frequency shift of  $1.5 \times 10^{-15}$ . Fortunately, we have sufficient optical power that it is not necessary to operate the AOM with this much RF power; instead, we typically use 30 dB less. While the long-term behavior (between 0.2 s and 1 s) shows that the phase chirp scales linearly with the RF power, the initial chirp (out to  $\sim 150$  ms) showed weaker scaling. As such, we conservatively place a  $1.5 \times 10^{-17}$  error bar on this effect.

Looking ahead to the next evaluation, it will be necessary to revisit this effect to see how it behaves with Ramsey interrogation. Particularly, how does the phase evolve during the dark time, when the RF is turned off? A different way to tackle this problem is to implement phase-stabilization, not just up to the tip of the optical fiber, but all the way to the optical lattice. In this case, the phase chirp associated with the AOM is just part of the total phase noise that is actively canceled by making suitable corrections to an AOM [206]. Because the Ramsey pulses are not especially short (10 ms or perhaps longer), pulsing the light on and off should not present too great a technical challenge in implementing such a servo, although care will need to be taken to ensure the phase excursions are not too large during the earliest part of the pulse before the servo has a chance to update.

#### 7.1.4 Residual Doppler effects

As discussed in Ch. 2, tight confinement in a harmonic potential strongly suppresses the Doppler effect, since the atom spends as much time moving toward the clock laser as away from it. However, this suppression breaks down for any excess motion which is correlated with the timing

of the clock spectroscopy [108, 36]. As a part of the clock stability measurements of Sec. 3.6, we considered noise arising from differential phase fluctuations between the clock light and the lattice light, and found it contributed to the instability at a level of  $1\text{--}2\times 10^{-16}$  (for 1-s averaging). These noise processes were thought to be due to air fluctuations and table vibrations, which, in general, should average to zero and cause no net frequency shift. But, this averaging breaks down for any correlated motion; one example of prime concern is that turning off the quadrupole magnetic field coils shakes the mechanical platform on which the optics are mounted, and because the coils are turned off at precisely the same moment (about 30 ms) before beginning clock spectroscopy, the effect might not fully average away. Here, we benefit from long interaction times, which further separate (in time) the clock spectroscopy from the shaking effects. Still, the possibility of a frequency shift warrants some investigation.

To look for this effect, we made two sets of timing measurements relative to the Ca clock. In the first, we changed the amount of ‘dead’ time between shutting off the coils and beginning spectroscopy. In one case, this time was the typical  $\sim 30$  ms, while in the other it was 150 ms longer. We also changed the Rabi probe time from 80 ms to 70 ms. The measurement result showed a difference between the two cases of  $19(25) \times 10^{-17}$  — statistically consistent with no shift.

The second measurement was similar. Here, we changed the duration of the Rabi pulse, as well as the amount of ‘dead’ time after spectroscopy but before detection. The two values for the Rabi pulse time were 80 and 40 ms, while the two values for the wait time after spectroscopy were 6 and 46 ms. As such, the total cycle time was preserved, but the window in which the atoms were illuminated was shortened. Note that this measurement also requires changes to the AOM’s RF power and to the optical power illuminating the atoms, in order to make a  $\pi$ -pulse in both cases. Here the differential shift between the two conditions was  $6(14)\times 10^{-17}$ .

While neither measurement is a completely thorough test capable of ruling out any correlated motion effects, we were pleased to see that both measurements showed null results at approximately the level of the clock’s total uncertainty budget. Since completing the 2009 evaluation, we have observed an interesting spectral effect that seems to be related to the idea of correlated motion.

When we slightly overdrive the Rabi pulse, the lobes of the  $\text{sinc}^2$  function become more prominent, and we observe slight asymmetry in the size of these features. Changing the duration of the Rabi pulse changes which side (red or blue detuning) has the taller feature. After studying this effect for some time, we reached the conclusion that it was most likely due to shaking of the mechanical platform, writing differential noise onto the lattice and clock beams. This will need to be studied more carefully in the future. Doppler effects such as these could be suppressed either by extending the path noise cancelation all the way to the lattice (so that the clock light is referenced to the rest frame defined by the lattice), or by implementing a bi-directional probing scheme [173] that alternates the direction of the probe light  $\vec{k}$  vector relative to the lattice.

Another effect to mention is the second-order (relativistic) Doppler effect. The fractional frequency shift is

$$\frac{\Delta\nu}{\nu_0} = \frac{1}{2} \frac{\langle v^2 \rangle}{c^2} \quad (7.2)$$

where the angle brackets denote a time-average. At these ultracold temperatures, the RMS velocity is only a few centimeters per second, and the associated frequency shift is below  $10^{-18}$ .

### 7.1.5 Servo error and line pulling

Servo error encompasses any effect that prevents the feedback loop from locking to the exact center of the atomic resonance. One main culprit is uncompensated linear drift of the reference cavity, which leads to an offset in the error signal of the feedback loop. We previously measured that a drift of 1 Hz/s causes a frequency shift of 2 Hz [90]. By implementing a second integrator, the drift rate of the first integrator is essentially zero; moreover, a manually adjustable feed-forward allows the clock operator (usually a graduate student) to act as a third integrator, updating the drift-canceling rate every few minutes to hold the second integrator value near zero. As such, we find the uncompensated drift rate to be  $< 0.1$  mHz/s, and the frequency offset is below 1 mHz.

Other servo errors result from round-off error in the digital servo and frequency noise near the modulation frequency ( $\sim 2$  Hz), but these are expected to be small effects. We have tested that

the micro-processor and DDS (recall Fig. 3.7) can accurately reproduce frequencies at the 1 mHz level.

Line-pulling can occur when any spectral features other than the carrier (i.e. motional sidebands,  $\sigma$ -transitions, or residual  $\pi$ -excitations from the opposite spin state) are unbalanced. Both the longitudinal and transverse motional sidebands are strongly suppressed during normal clock operation due to the strong confinement and well-aligned probe beam. The  $\sigma$ -transitions are largely suppressed (by a factor of  $\sim 5$  compared to  $\pi$ -transitions) by optical polarization, while  $\pi$ -excitation from the opposite spin state is no more than 1 % because of the spin-polarization fidelity. Even assuming worst-case scenarios in how imbalanced the red- and blue-detuned features are, none of these effects is expected to cause line-pulling at the  $10^{-18}$  level. This is in large part due to the narrow-line spectroscopy, which cleanly resolves the carrier transition from all other spectral features.

#### 7.1.6 DC Stark shift from stray charge

Any stray charge that accumulates on dielectric surfaces near the atoms creates an electric field and a Stark shift. Because the atoms are held in an optical potential, there is very little dielectric matter nearby on which stray charge can accumulate. Perhaps the only concern is any charge that accumulates unevenly on opposing vacuum viewports, though these are  $\sim 5$  cm from the atoms. In one apparatus [246], very large Stark shifts were associated with stray charge; however, we note that this apparatus used a build-up cavity inside the vacuum chamber, and one of its mirrors was mounted on a PZT with a high voltage connection. This apparatus is thus very different from the one considered here.

In Ch. 6, we applied a large electric field and reversed its direction, leading to a direct observation of stray fields on the order of 0.1 V/cm, although these could have been caused by differential contact potentials instead of stray charge. Of course, this measurement was only sensitive to the projection of the stray field onto the electrode axis ( $\vec{E}_s \parallel \vec{E}_a$ ). Fortunately, with numerical modeling, we find that any stray charge, sprayed onto the vacuum viewports, creates a field with at

least a 10–20 % projection onto the electrode axis. Thus we can already constrain the stray field to below 1 V/cm, for which an upper limit to the d.c. Stark shift is  $8 \times 10^{-18}$ . But fields this large seem unlikely. With stand-off voltage sensors, it may be possible to constrain the potential on the dielectric surface to less than 1 V, corresponding to a field of order 0.1 V/cm, and at this level the d.c. Stark shift is below  $1 \times 10^{-18}$ . Alternatively, the conductive enclosure that will be used to shield the atoms from stray blackbody radiation (Sec. 6.4) would also ensure that stray fields are negligibly small.

### 7.1.7 Systematic totals

Table 7.1 gives a list of all known systematic effects and their errors. The left side of the table lists the results from the 2009 evaluation [43], showing a total systematic uncertainty of  $3.4 \times 10^{-16}$  and indicating the Yb lattice clock is (slightly) higher-performing than the best microwave clocks. As of this writing, this total remains among the lowest reported for any lattice clock system [72, 49], though a few ion clocks have reported lower numbers [36, 37, 247].

The right side of the table shows progress toward a re-evaluation that is currently underway. Effects that have been measured or calculated are shown in black. For the remaining effects, the red text corresponds to a reasonable upper limit to the uncertainty associated with that effect. The biggest leap is to assume that the lattice effects (Ch. 4) can be controlled at or below the  $10^{-17}$  level. However, with the improvements to clock stability, decoupling of density shifts, and the possibility of a build-up cavity to increase the lever arm, this ought to be straightforward. Other effects that require further attention are the AOM phase chirp and residual Doppler effects, as described above. The Zeeman sensitivities could benefit from further measurement, but here it is instead assumed that the field was reduced by a factor of 5 with no re-measurement.

As is clear from the table, the clock’s uncertainty is directly reduced by the measurement efforts described in Ch. 5 and Ch. 6 to control density-dependent and blackbody shifts. If the lattice light shift measurements produce similar results (as we expect they will), the total clock uncertainty will soon be just a few parts in  $10^{17}$ , a level which has yet to be achieved by any neutral



Table 7.1: Uncertainty budget for systematic effects in the  $^{171}\text{Yb}$  optical lattice clock. Values are given in fractional units  $10^{-17}$  and represent typical operating conditions. The results of the 2009 evaluation are shown at the left, leading to a reported systematic total of  $3.4 \times 10^{-16}$ . At the right, progress toward a re-evaluation (in progress) is shown. Effects that have been measured are given in black text, while the red text gives a reasonable upper limit for the uncertainty associated with effects which require further measurement.

| Effect                        | Shift      | Uncertainty | Shift      | Uncertainty |
|-------------------------------|------------|-------------|------------|-------------|
|                               | (ca. 2009) |             | (ca. 2012) |             |
| Blackbody                     | -250       | 25          | -246.3     | 3.4         |
| Density-dependent             | -161       | 8           | 0.5        | 0.5         |
| Lattice scalar                | 4          | 17          |            | 1           |
| Lattice hyperpolarizability   | 33         | 7           |            | 1           |
| Lattice multipolar            | 0          | 10          |            | 1           |
| 1 <sup>st</sup> -order Zeeman | 4          | 4           | 0.8        | 0.8         |
| 2 <sup>nd</sup> -order Zeeman | -17        | 1           | -0.7       | 0.3         |
| Probe light                   | 0.5        | 1           | 1          | 0.6         |
| AOM phase chirp               | 0          | 1           |            | 0.5         |
| Servo and line pulling        | 0          | 1           | 0          | 0.1         |
| Residual Doppler              | 0          | 1           |            | 0.5         |
| d.c. Stark shift              | 0          | 1           | 0          | 0.8         |
| Total                         | -387       | 34          |            | 4.1         |

atom clock. Importantly, future clock frequency measurements (relative to Cs or other optical clocks) will likely require only two substantial corrections — those due to blackbody radiation and hyperpolarizability.

## 7.2 Absolute frequency measurement with NIST-F1

We made a series of absolute frequency measurements by comparing the Yb clock frequency to the Cs fountain clock NIST-F1. Here, the frequency comb's repetition rate is locked to the Yb-stabilized laser. A photodetector outputs an electronic signal at  $f_{\text{rep}} \approx 1$  GHz, and a synthesizer is used to mix down this signal to low frequency, where it is counted. The synthesizer and the counter are referenced to the 10-MHz hydrogen maser signal that also provides the (long-term) LO for the atomic fountain clock. As shown in Fig. 7.4, long averaging times (many hours) are required to make frequency measurements near the  $10^{-15}$ -level. The role of the fountain clock is to provide a

calibration of the hydrogen maser frequency, from which we can determine the Yb clock frequency. The maser corrections (“steers”) are encoded as a frequency offset with a digital synthesizer, sent by cable from the fountain lab to the comb lab (a few hundred meters away), and counted in real time. We made three measurements in this manner, each lasting 12–24 hours; the results are shown as blue points in Fig. 7.5.

The maser can also be calibrated relative to the NIST timescale, which is useful if the Cs fountain is not simultaneously running. Ultimately the correction is derived from Cs measurements, but in a less direct manner, and is determined as an average over a several hour measurement time. Maser corrections determined in this way come with extra uncertainty, but are nonetheless useful for determining the absolute frequency. The green points in Fig. 7.5 were measured using this average maser correction technique.

Regardless of which technique is used to calibrate the maser, it is also necessary to correct for the gravitational redshift between clocks at differing gravitational potentials. Near earth’s surface, we can treat the gravitational acceleration ( $g \approx 9.8 \text{ m/s}^2$ ) as a constant, and the fractional redshift is given by the height difference ( $\Delta h$ ) between the two clocks:

$$\frac{\Delta\omega}{\omega_0} = \frac{g \Delta h}{c^2}. \quad (7.3)$$

This results in a shift of  $1.1 \times 10^{-16}$  per meter of height difference. Between NIST-F1 and the Yb atoms, we measured  $\Delta h \simeq 300(10) \text{ cm}$ , leading to a shift of 0.17 Hz with negligible uncertainty. In this case, the Yb clock was located above the Cs fountain, where gravity is weaker, meaning that the observed Yb frequency should be reduced by 0.17 Hz.

The first four measurements in Fig. 7.5 have a mean of 518 295 836 590 865.2(7) Hz, and this result was published in [43]. The full record of 11 measurements gives 518 295 836 590 865.0(5) Hz, with  $\chi^2_{\text{red}} = 1.15$ . The red lines in the figure show this mean and 1- $\sigma$  error bars. Subsequent to these measurements, two other laboratories have measured the Yb clock frequency and found good agreement, though with somewhat larger uncertainties [76, 249].

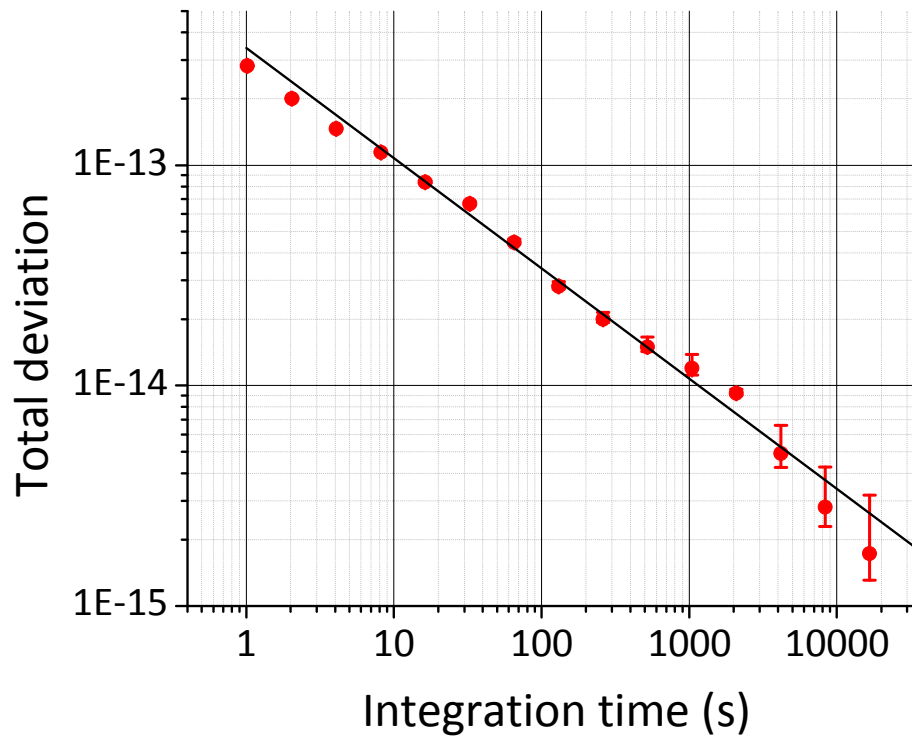
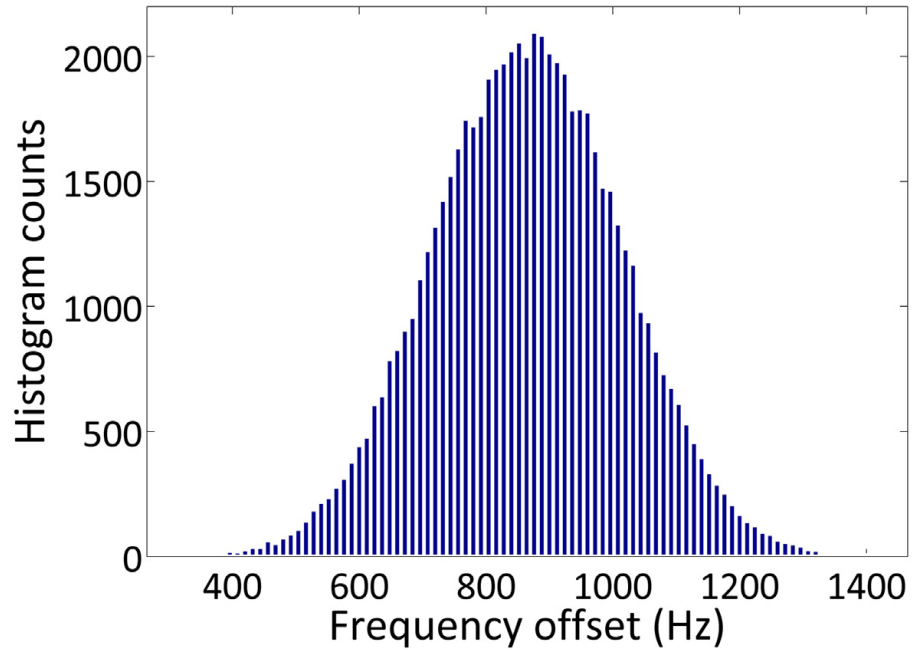


Figure 7.4: A histogram and the total deviation (similar to the Allan deviation [248]) are used to characterize the frequency stability between the Yb clock and the hydrogen maser. In the lower figure, the solid line gives the frequency instability as  $3.4 \times 10^{-13}/\sqrt{\tau}$ .

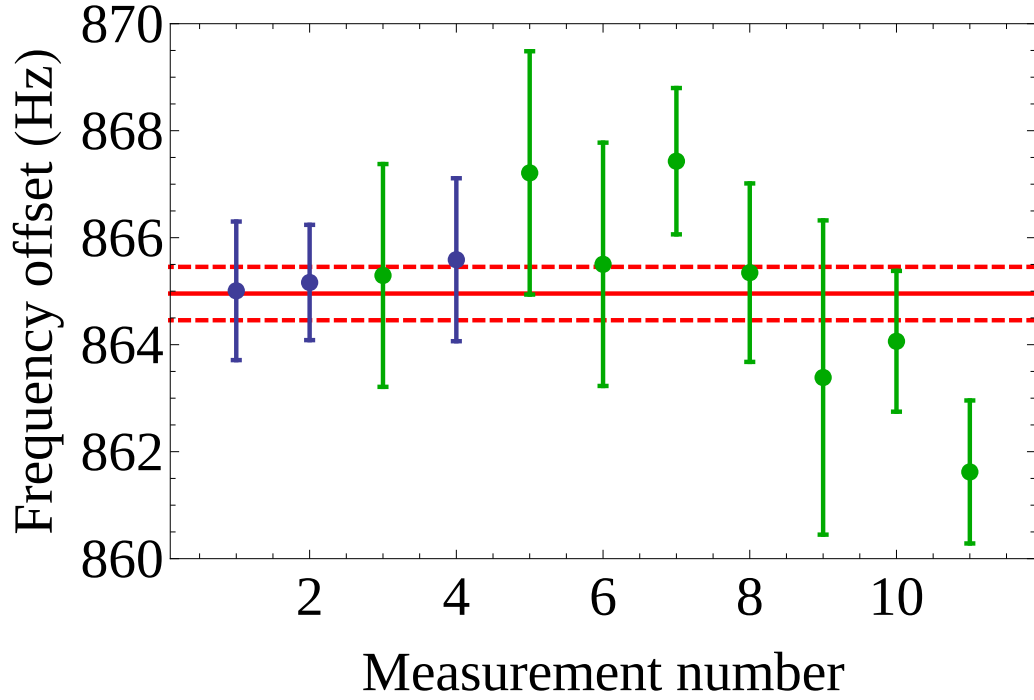


Figure 7.5: From 2008 to 2010, we performed a series of measurements with the Cs fountain clock NIST-F1. The frequency determined from each measurement is plotted; blue points use the “steers” counting technique, while green points use the average maser correction technique. The red lines show the mean and 1- $\sigma$  error bars. From these 11 measurements, we find the frequency to be 518 295 836 590 865.0(5) Hz, with  $\chi^2_{\text{red}} = 1.15$ .

### 7.3 Conclusion

As we come to the end, it's worthwhile to recall where we've been. While the Yb clock's performance can largely be summarized with its systematic uncertainty (Table 7.1) and its estimated stability (Fig. 3.10), some of the most interesting physics is not encompassed by these numbers.

This includes the studies of density-dependent shifts to identify  $p$ -wave collisions between the Yb atoms, a result which was somewhat surprising given previous work with Sr atoms [128] and the ensuing theoretical descriptions [209, 208, 210]. One counterintuitive result of this work was that strong interactions can actually lead to smaller frequency shifts, as discussed in Sec. 5.5. Similarly, our observation of inelastic loss processes was an interesting and unexpected discovery.

The polarizability measurements of Ch. 6 yielded not only a number ( $\alpha_{\text{clock}}$ ) with very small uncertainties, but also the opportunity to make a precise measurement of something other than a frequency (in this case, the applied electric field,  $E_a$ ). One pleasantly surprising result of this effort was that the final uncertainty was lower than we initially planned for and was dominated by the possible error in the voltmeter, something that could easily be reduced with access to a higher-performance voltage standard. The technique we employed could be applied to other lattice clock atoms (Sr [225] and Hg), which would be useful not only for metrologists but also for atomic structure theorists.

Finally, observing a Rabi spectrum with a 1 Hz linewidth was an exciting accomplishment, it being the highest demonstration of coherent spectroscopy to date. It's good for that title to be held by a lattice clock, since it will likely be quite some time before any lattice clock equals the current performance of the best ion clocks in terms of total systematic uncertainty.

### 7.4 Outlook

From the perspective of basic science, hopefully the research contained in this thesis (and, generally, the research undertaken worldwide by lattice clock-makers) has merit independent of any scientific and technological applications to which it may lead. Still, it's also exciting to look

ahead and wonder what the next decade holds for time and frequency measurements. The “race” to re-define the SI second in terms of an optical transition is clearly underway, although many other technological pieces (including improved methods for intercontinental frequency comparisons and a higher-stability timescale) must also be solved before any of the benefits of an optical realization of the second can be enjoyed.

As mentioned in Ch. 1, the two main technologies competing to be the next primary standard are single ion clocks and lattice clocks. While the highest-performing lattice clocks still trail the highest-performing single ion clocks by a substantial margin in total systematic uncertainty [36, 37], we should also consider not just the absolute best results that have been obtained, but also the results of other groups working with the same systems. No groups outside of NIST, to this author’s knowledge, have yet demonstrated a functioning  $\text{Hg}^+$  or  $\text{Al}^+$  ion clock at any level, though in the latter case there is work underway in at least one other institute [250]. By contrast,  $^{171}\text{Yb}$  lattice clock has been measured relative to the cesium frequency in three laboratories [43, 76, 249], while the  $^{87}\text{Sr}$  lattice clock remains the best characterized optical frequency standard thanks to the contributions of many groups [251, 252, 136, 49]. Other ion clocks, including  $\text{Yb}^+$  and  $\text{Sr}^+$ , remain candidates as well, and may be experimentally simpler alternatives to  $\text{Al}^+$ . As for lattice clocks, neutral Hg remains in the mix thanks to its reduced sensitivity to blackbody radiation [80], although the experiments carried out thus far seem quite challenging [253]. We should also note that different kinds of clocks may be able to meet the needs of different applications. After all, the laboratory environment is significantly different from that of a satellite.

Within the lattice clock field, it seems that nearly all groups are currently pursuing fermionic isotopes (specifically  $^{87}\text{Sr}$ ,  $^{171}\text{Yb}$ , and  $^{199}\text{Hg}$ ). However, bosonic systems could be competitive, especially with the reduced spectroscopic shifts afforded by narrower lines [85] and tailored Ramsey pulse sequences [254]. A related question is what dimension of lattice confinement will ultimately produce the highest performance. One leading figure in the lattice clock field has recommended [91] that fermionic (odd isotope) systems should use 1D confinement, where the vector and tensor shifts are not problematic, while bosonic (even isotope) systems should use 3D confinement to

suppress the potentially large collision shifts [73].<sup>2</sup> After subsequent work showed both fermionic Sr and Yb had non-zero collision shifts, it seemed that fermionic systems would also require higher dimensional confinement; but the most recent work with fermionic Sr in a 2D lattice [256] as well as our work with fermionic Yb in a 1D lattice [213] has shown that collision effects can be minimized even with more than one atom per lattice site. While there's perhaps something most satisfying about deep confinement in all three dimensions, no 3D lattice clock has been demonstrated with a total systematic uncertainty near to those of the best 1D clocks [219, 1].

As for the spin-1/2 Yb clock described in this work, the outlook remains positive. With a cryogenic shield surrounding the atoms, perhaps the BBR uncertainty could be as small  $1 \times 10^{-18}$ ; in this case, a whole host of other systematic effects must be characterized to the same level, but to date no obstacles have been identified. Higher  $Q$ -factors and better short-term stability will be essential, and these may require new ideas for how to produce a low-noise LO [177, 178, 182, 181]. And what could be more fun than investigating new ideas?

In addition to pushing lattice clocks to higher levels of stability and repeatability, several other goals should be worked towards. For one, there has never been a high-level measurement of the ratio of two lattice clock frequencies, as there has for  $\text{Al}^+$  and  $\text{Hg}^+$ . Such a measurement could demonstrate the performance of lattice clocks in a manner that internal evaluations simply cannot. With neutral Hg still in its formative years as a frequency standard, the most likely measurement would be Yb – Sr. With new optical links in place throughout the European continent and between several institutes in Japan, this ratio could be measured on three continents, including here in Boulder. Showing agreement at or below the  $10^{-15}$  level would be a good start, while the  $10^{-16}$  level would be a major accomplishment. While the lack of a discrepancy between measurements of the same atoms might not make international headlines or win new prizes for the experimentalists, I believe it's an essential step before lattice clocks can really be trusted at the levels we claim they

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<sup>2</sup> Interestingly, our work with bosonic  $^{174}\text{Yb}$  resolved no collision shift at the  $10^{-15}$  level. Now that we have developed the tools for observing very fine details of the collisional effects, we should revisit this measurement. It's always possible that the relevant scattering lengths could fortuitously cancel the frequency shift, as in  $^{87}\text{Rb}$  [255], which would be an important discovery.

can.

A second goal is to develop field deployable clocks. Here again, this effort might not be ripe with new physics to uncover, but (speaking as a physicist) it would be disappointing if all the new science that has been uncovered cannot be harnessed into something more useful than a room-sized device that measures the time of day. Indeed, some of the most exciting prospects for lattice clocks involve carrying them into space to see what happens to their frequencies, but currently most lattice clocks are nowhere near being ready for deployment.

The next decade promises to be the heyday of optical clocks, and due to their worldwide proliferation, lattice clocks will clearly be a key component. But with an eye to the future, we should remember what makes optical clocks so precise — their incomprehensibly high frequencies — and take note that maybe it might not be long before even higher frequency clocks (such as the low-lying nuclear clock transition in  $^{229}\text{Th}$  [257, 258, 259, 260]) become a reality.



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## Appendix A

### Calculating atomic density

#### A.1 One-dimensional lattice

In the laboratory we measure the following quantities: total number of atoms  $N_{tot}$ , trap frequencies  $\omega_i$  for  $i = \{x, y, z\}$ , temperature  $T$ , and  $1/e$  spatial extent along the lattice direction  $\sigma$ . Here we show how to use these measurements to find the density of each site  $\rho_k$  for  $k$  the index of the lattice site, the average number of atoms per lattice site  $\bar{N}$  (spatially-averaged over all sites), and the spatially-averaged density  $\bar{\rho}$ .

We begin by assuming that atoms fill the lattice with a Gaussian distribution:

$$N(k) = \frac{N_{tot} \lambda}{2\sqrt{\pi}\sigma} e^{-\left(\frac{k\lambda}{2\sigma}\right)^2} \quad (\text{A.1})$$

where the pre-factor in front of the exponential function comes from normalization, and  $\lambda$  is the lattice wavelength. Because there are more than 1000 sites we treat  $k$  as a continuous variable. In general, to evaluate an expectation value of a quantity  $A(k)$ , we integrate along this distribution:

$$\bar{A}(k) = \frac{\int A(k)N(k)dk}{\int N(k)dk} \quad (\text{A.2})$$

So to find the average number of atoms per lattice site, this becomes

$$\bar{N} = \frac{\int N(k)^2 dk}{N_{tot}} = \frac{N_{tot}\lambda}{2\sqrt{2\pi}\sigma} \quad (\text{A.3})$$

Now we turn to calculating the volume part of the density. From the temperature and trap frequency measurements, we can find thermally-averaged mode numbers:

$$\langle n_i \rangle = \frac{1}{e^{\frac{\hbar\omega_i}{k_B T}} - 1} \quad (\text{A.4})$$

where  $k_B$  is the Boltzmann constant. Next we can find characteristic length parameters  $\langle L_i \rangle$  by setting the total energy of the harmonic oscillator equal to the potential energy evaluated at the classical turning point, which yields

$$\langle L_i \rangle = \sqrt{\frac{\hbar (2 \langle n_i \rangle + 1)}{m \omega_i}} \quad (\text{A.5})$$

with  $m$  the atomic mass. Note that  $\langle L_i \rangle$  scales nearly linearly with  $\omega_i$ . Next we assume Gaussian-distributed density along all 3 spatial dimensions within a given lattice site:

$$\rho_k(x, y, z) = N(k) \frac{1}{\sqrt{\pi} \langle L_x \rangle \sqrt{\pi} \langle L_y \rangle \sqrt{\pi} \langle L_z \rangle} e^{-\left(\frac{x}{\langle L_x \rangle}\right)^2 - \left(\frac{y}{\langle L_y \rangle}\right)^2 - \left(\frac{z}{\langle L_z \rangle}\right)^2} \quad (\text{A.6})$$

To calculate the spatially-averaged density within lattice site  $k$ , we integrate as in Eq. A.2

$$\rho_k = \frac{1}{N(k)} \int \rho(x, y, z)^2 dx dy dz \quad (\text{A.7})$$

$$\rho_k = \frac{N(k)}{(2\pi)^{3/2} \langle L_x \rangle \langle L_y \rangle \langle L_z \rangle} \quad (\text{A.8})$$

Combining Eqs. A.3 and A.8 we can find the average density over the entire lattice  $\bar{\rho}$

$$\bar{\rho} = \frac{N_{tot} \lambda}{8\pi^2 \sigma \langle L_x \rangle \langle L_y \rangle \langle L_z \rangle} \quad (\text{A.9})$$

For our 1-D lattice parameters we find the following:

$$T = 10.5 \text{ } \mu\text{K}$$

$$N_{tot} = 2.6 \times 10^4 \text{ (for 1000 "atom counts")}$$

$$\lambda = 759 \text{ nm}$$

$$\sigma = 186 \text{ } \mu\text{m}$$

$$\omega_x = \omega_y = 2\pi \text{ } 575 \text{ Hz}$$

$$\omega_z = 2\pi \text{ } 85 \text{ kHz}$$

$$\langle n_x \rangle = \langle n_y \rangle = 380$$

$$\langle n_z \rangle = 2.1$$

$$\langle L_x \rangle = \langle L_y \rangle = 9 \text{ } \mu\text{m}$$

$$\langle L_z \rangle = 60 \text{ nm}$$

$$\overline{N} = 21$$

$$\overline{\rho} = \rho_1 = 2.9 \times 10^{11}/\text{cm}^3$$

It's also instructive to consider how the temperature  $T$  and density  $\rho$  of the trapped ensemble varies with the trap depth  $U_0$ . One can imagine three cases, depending on the final temperature of the 556 nm MOT ( $T_{\text{MOT}}$ ):

a)  $T_{\text{MOT}} \ll U_0$

If the full Boltzmann distribution lies below the lattice potential depth, then in principle all of the atoms could be trapped, and the temperature is independent of (small) changes in  $U_0$ . However, the density does depend on the trap depth, as higher depths more tightly confine and compress the atoms. For a fixed temperature, the characteristic oscillator length of the trapped ensemble scales as  $1/\omega_i$  for each dimension  $i = \{x, y, z\}$ , leading to a scaling  $\rho \propto U_0^{3/2}$ .

b)  $T_{\text{MOT}} \gg U_0$

In the opposite extreme, the lattice depth is much lower than the atomic temperature. In this case, the Boltzmann distribution is truncated, and the distribution of occupied motional states no longer follows Maxwell-Boltzmann statistics. Nonetheless, if we assigned a temperature, we expect  $T \propto U_0$ , as a deeper trap could confine warmer atoms, thereby raising the average temperature of the confined sample. Because the characteristic harmonic oscillator length in each dimension scales as  $\sqrt{T} = \sqrt{U_0}$ , the combined density scaling (including the change in confinement described above) all cancels out. That is, the density is independent of small changes in  $U_0$ .

c)  $T_{\text{MOT}} \sim U_0$

In the intermediate regime, which is most applicable to the Yb experiment, we expect intermediate strength scaling:  $T \propto \sqrt{U_0}$ . In this case, the density scales as  $\rho \propto U_0^{3/4}$ . We use this expected scaling when comparing collision shift experiments performed at slightly different trap depths.

## A.2 Two-dimensional lattice

In our 2D lattice, we estimate that 7,000 atoms remain in the trap after the “filtering” step (Sec. 3.2.2), or about four times fewer than the 1D lattice. However, the number of lattice sites is increased dramatically. With a  $1/e$  intensity radius of  $\sim 30 \mu\text{m}$  and a lattice spacing of  $\approx 380 \text{ nm}$ , the number of sites is approximately 25,000. Under these conditions, we would expect the majority of atoms to be in singly-occupied lattice sites.

We can estimate the fraction of multiply-occupied lattice sites with a simple model. Taking the lattice as a grid of  $L$  total sites, we can start filling it with atoms one at a time. For the  $i^{\text{th}}$  atom, the odds of landing in a filled site are

$$P_2(i) = \frac{i-1}{L}. \quad (\text{A.10})$$

When summed to the total atom number  $A$ , we obtain the number of doubly-occupied sites ( $N_2$ )

$$\begin{aligned} N_2 &= \sum_{i=1}^A P_2(i) \\ &= \frac{A(A-1)}{2L} \end{aligned} \quad (\text{A.11})$$

and the fraction of atoms in doubly-occupied sites ( $F_2$ )

$$\begin{aligned} F_2 &= \frac{2N_2}{A} \\ &= \frac{A-1}{L}. \end{aligned} \quad (\text{A.12})$$

Similarly, we can find the fraction of atoms in sites with three and four atoms:

$$\begin{aligned} F_3 &= \frac{3}{A} \sum_{k=1}^A \frac{1}{L} N_2(k) \\ &= \frac{A^2-1}{2L^2} \\ F_4 &= \frac{4}{A} \sum_{j=1}^A \frac{1}{L} N_3(j) \\ &= \frac{A^3+2A^2-A-2}{6L^3} \end{aligned} \quad (\text{A.13})$$

We can compare these estimates to a Monte Carlo simulation of the lattice filling (Fig. A.1). As is shown in the figure, the simple model does a good job predicting the filling at low atom

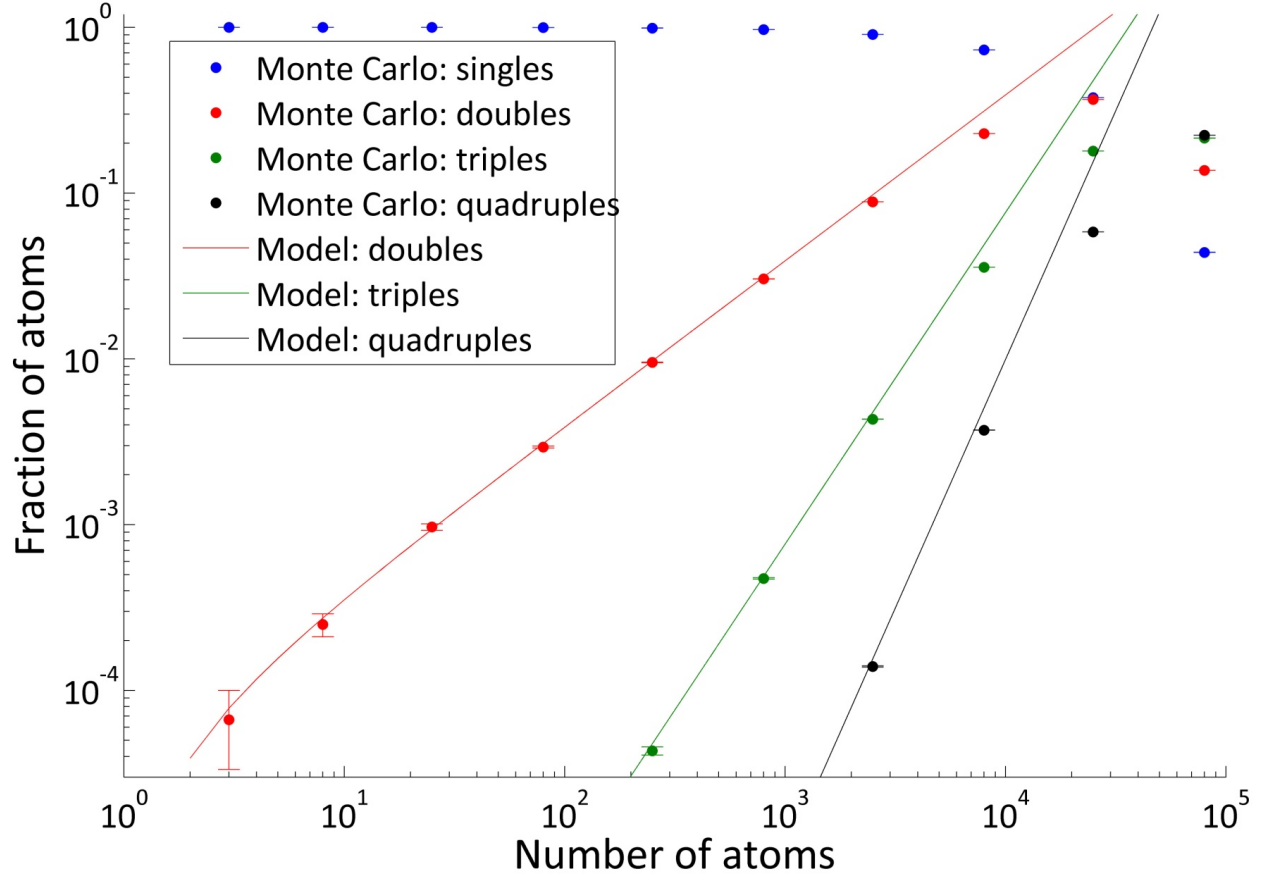


Figure A.1: The markers show the results of a Monte Carlo simulation that randomly fills the 2D lattice with atoms and counts the fraction in singly- and multiply-occupied tubes. Here, the number of lattice sites was taken to be  $L = 160^2 \approx 25,000$ . The solid lines show the prediction of the simple model presented in the text. As expected, the model performs best for smaller atom numbers, where  $F_1 \gg F_2 \gg F_3 \gg F_4$ .

number ( $A < L$ ). At higher filling fractions, the model should be corrected for the fact that each triply-occupied site actually depletes the number of doubly-occupied sites, and so on. For our parameters,  $L \approx 25,000$  and  $A \approx 7,000$ , we find 73 % of the atoms are in singly-occupied sites, 23 % in doubly-occupied sites, and 4 % in triply- or higher-occupied sites.

In the 1D case we treated the effective size of each lattice site as identical, which is well-justified considering that the Rayleigh range of the lattice beam exceeds the  $1/e$  extent of the trap by an order of magnitude. However, it was important to spatially average over the number of atoms in each site. By contrast, in the 2-D case we consider only those lattice sites which have multiple atoms (since singly occupied sites have no atom-atom collisions), the majority of which have only two. However, the details of the confinement (and hence the volume part of the density) vary across the lattice because of the 2-D Gaussian shape.

As an estimate, we consider a lattice site near the center of the trap. The number of atoms is reduced from the 1-D case by a factor of 10, but the trap frequency along  $y$  is increased by a factor of 100 (from  $\sim 600$  Hz to  $\sim 60$  kHz). This reduces  $\langle L_y \rangle$  by nearly the same factor of 100. These two effects give us a factor of 10 increase in  $\bar{\rho}$ , leading to an estimated density of  $\rho_2 = 4 \times 10^{12}/\text{cm}^3$  as mentioned in Ch. 5.