Chapter 1: Introduction

Why is quantum simulation important:

- Can help understand problems that are not easy to solve numerically or analytically. High temperature superconductors, frustrated systems, as good examples.

- Create analogues to systems that would otherwise not be possible to study. Example: the expanding universe, Hofstadter at large magnetic fields.

- Create new exotic systems that do not exist in nature but can help us learn or understand something... or are just fun!

Don't forget to talk about topology! It starts with condensed matter but has been relevant to many other systems. Many Noble prizes awarded, many applications and potential applications found.

Start with topology and move into quantum simulation? Or the other way around?

1.1   Thesis overview

In Chapters 2 and 3 I will describe the basic theory of Bose-Einstein condensation and the technical details of our experimental apparatus that produces ^{87}Rb BECs. In Chapter 4 I will describe our quantum simulation toolkit, the standard techniques that we use to manipulate and detect ensembles of ultracold atoms that are necessary for all of our experiments. Chapter 5 describes a Fourier transform spectroscopy technique that exploits the relation between quantum coherent evolution and the underlying spectrum of a system and that was used to characterize experiments described later in the thesis. Chapter 6 describes an implementation of continuous dynamical decoupling that helped to both make our system more robust against environmental noise and also allowed us to couple the internal states of the atoms in new ways that were not possible before, opening the path for new kinds of quantum simulations described in Chapters 7 and 8. In Chapter 8 I describe the experimental realization of Rashba spin-orbit coupling for a quantum system without a crystalline structure and has unconventional topology characterized by non-integer topological invariants. Finally, Chapter 8 describes the experimental implementation of a fractional period adiabatic superlattice, an intermediate step

necessary for us to generate Hofstadter cylinders with non-zero magnetic flux in the future.

Apendix are experiments that I contributed to but are not included in the thesis. Also things related to new apparatus?

Chapter 2:   Basic theory of Bose-Einstein condensation

2.1   The Bose-Einstein distribution

2.2   BEC transition and critical temperature

2.3   BEC in a harmonic potential

2.4   BEC with interactions

2.4.1   GPE equation

2.4.2   Thomas-Fermi approximation

Why the BEC has the shape of an inverted parabola.

2.4.3   Expansion of atomic cloud in 3D harmonic potential

How one can infer atomic densities and temperature (from thermal atoms) from time of flight images.

Chapter 3:   Coherent manipulation and detection of ultra-cold atoms

All of the experiments described in this thesis were performed using ultracold clouds of ^{87}Rb. Both the cooling and trapping of atoms as well as the engineering of potentials and detection of atoms rely on the interaction of atoms with electromagnetic fields as well as with static and oscillating magnetic fields.

In this Chapter I will describe the techniques and interactions that make our experiments possible. I will start by describing the electronic structure of ^{87}Rb. I will review the effects of the atomic interactions with magnetic and electric fields. First I will talk about the foundations of atom-light interactions that make possible both laser cooling and trapping and Raman induced transitions. I will then talk about the interactions of atoms with magnetic fields which allows us to shift the energies of different atomic states and . Finally I will discuss the absorption imaging technique that we use to detect atoms after all our experiments are performed.

3.1   Electronic structure of ^{87}Rb

Rb is an Alkali metal (also Li, which exists in our vacuum chamber but was never used). Alkali metals correspond to the first group (leftmost column) of the periodic table and are characterized by having a single valence electron, which makes the description of their internal structure much simpler than that of other elements. We can describe the state of an electron in an atom by its angular momentum $\hat{\mathbf{L}}$ and its spin $\hat{\mathbf{S}}$. Because of Pauli's exclusion principle there can not be two electrons with the same quantum numbers and in multi-electron atoms they tend to fill 'shells' of different angular momentum values, historically labeled by the letters S, P, D, F, ...[1] (corresponding to $L = 1$, 2, 3, 4, ...). In particular Rb has 4 filled shells and one electron in the $5S$ shell, where the number 5 corresponds to the principal quantum number n. Figure [TODO: make figure of atomic energy levels] shows the energy levels of the ground state $5S$ and its closest $5P$ orbital.

The atomic level structure is modified by relativistic effects. In particular the relativistic treatment of the electron's motion gives rise to an interaction between the electron's intrinsic magnetic moment (the spin) $\hat{\mathbf{S}}$ and the orbital angular momentum $\hat{\mathbf{L}}$. This spin-orbit coupling interaction $\hat{H}_{\text{fs}} \propto \mathbf{L} \cdot \mathbf{S}$ causes the fine structure splitting of the electronic orbitals into levels with different total electronic angular momentum $\mathbf{J} = \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$. Figure **??**b show the $5^2 S_{1/2}$, $5^2 P_{1/2}$ and $5^2 P 3/2$ electronic configurations

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[1] This terms were used to describe the lines in the emission spectra when they were first discovered. S stands for sharp, P for principal D for diffuse and F for further noted

that arise from this splitting, where the subscript indicates the value of J. For S ($L = 0$) orbitals $J = 1/2$ is the only possible value and the levels are not split. For the P orbital ($L = 1$) J and a single electron with $S = 1/2$, J can be $1/2$ or $3/2$ and the P orbital splits into two levels. The $5S_{1/2} \rightarrow 5P_{1/2}$ is known as the D1 line and has wavelength $\lambda = 794.979\,\mathrm{nm}$ and $5S_{1/2} \rightarrow 5P_{3/2}$ transition is known as the D2 line and has $\lambda = 790.241\,\mathrm{nm}$ [1].

The atomic level structure gets further modified by the magnetic interaction of the electronic magnetic flux density with the nuclear spin **I**. This is another kind of spin-orbit interaction that gives rise to the hyperfine splitting of the atomic levels which can be described by the Hamiltonian $\hat{H}_{\mathrm{hfs}} = A_{\mathrm{hfs}}\mathbf{I} \cdot \mathbf{J}$. A complete derivation of $\hat{H}_{\mathrm{hfs}}$ can be found in [2]. The hyperfine levels correspond to different values of the total angular momentum $\hat{F} = \hat{J} + \hat{I}$. For $^{87}\mathrm{Rb}$ $I = 3/2$ [1] which results in the level structure shown in Figure **??**c

3.2 Atom-light interaction

In this section I will discuss the interaction between atoms and electromagnetic radiation (light). After laying the foundations I will discuss the applications using off-resonant light such as optical dipole traps and Raman transitions. I will not cover laser cooling which has been covered extensively in the literature [3, 4] and PhD theses from previous lab members [5, 6].

In the presence of an electric field **E** an atom can become polarized and therefore its energy levels get modified by the Stark effect [7]. If the electric field is spatially uniform with respect to the atom's size we consider the electric field as a classical object and its effect on the atom can be described by the the Hamiltonian [8]

$$\hat{H}_{\mathrm{dip}} = -\hat{\mathbf{d}} \cdot \mathbf{E}, \tag{3.1}$$

where $\hat{\mathbf{d}} = -e \sum_j r_j$ is the atomic dipole operator, e is the electron charge and $\hat{r}_j$ are the position operators of the atom's electrons relative to the center of mas of the atom. This approximation, known as the dipole approximation, is valid for electromagnetic radiation when the wavelength is much larger than the size of an atom $\lambda \gg r_{\mathrm{atom}}$ [9].

For a coherent electromagnetic field $\mathbf{E}(\omega, t)$ with angular frequency ω, the dipole Hamiltonian can be written in terms of a dynamic polarizability

$$\hat{H}_{\mathrm{dip}} = -\alpha_{\mu\nu}(\omega)E_\mu^{(+)}E_\nu^{(-)} \tag{3.2}$$

where $\mathbf{E}^{(\pm)}$ are the possitive/negative frequency components of the field. $\alpha_{\mu\nu}(\omega)$ can be found by looking at the (time averaged) shift in the energy of the a given state state using second order time-dependent perturbation theory [9, 10]. For the ground state $|g\rangle$ the polarizability takes the form

$$\alpha_{\mu\nu}(\omega) = \sum_j \frac{2\omega_{jg} \langle g| d_\mu |e_j\rangle \langle e_j| d_\nu |e_j\rangle}{\hbar(\omega_{jg}^2 - \omega^2)}, \tag{3.3}$$

where $|e_j\rangle$ represent the excited states and $\omega_{jg} = (E_j - E_g)/\hbar$. The dipole operator is a rank-1 tensor and can be represented by 3 irreducible tensor operators[2] (see [9] for a complete derivation). In the limit of small magnetic fields so that F and m_F are good quantum numbers describing the state of the atom $|n, F, m_F\rangle$ the dipole Hamiltonian in this representation takes a convenient form

$$
\begin{aligned}
\hat{H}_{\text{dip}} = &\alpha^{(0)}(\omega)(\mathbf{E}^{(-)} \cdot \mathbf{E}^{(+)}) + \alpha^{(1)}(\mathbf{E}^{(-)} \times \mathbf{E}^{(+)}) \cdot \hat{\mathbf{F}} \\
&+ \alpha^{(2)} E_i^{(-)} E_j^{(+)} \left(\frac{1}{2}(F_i F_j + F_j F_i) - \frac{1}{3}\hat{\mathbf{F}}^2 \delta_{i,j} \right) \bigg],
\end{aligned}
\tag{3.4}
$$

where $\alpha^{(0)}$, $\alpha^{(1)}$ and $\alpha^{(2)}$ are the scalar, vector and tensor polarizabilities respectively and $\hat{\mathbf{F}}$ is the total angular momentum operator. For all our experiments $\alpha^{(2)}$ is very small so I will limit the discussion to the effect of the first two terms. The scalar term is responsible for the dipole force that allow us to trap atoms using off-resonant light and the vector component is necessary for engineering spin-orbit coupling through Raman transitions and other spin-dependent potentials.

3.2.1 Scalar polarizability

The scalar polarizability takes the form

$$
\alpha^{(0)} = \sum_j \frac{2\omega_{jg} \langle g| \mathbf{d} \cdot \hat{\epsilon} |e_j\rangle |^2}{\hbar(\omega_{jg}^2 - \omega^2)},
\tag{3.5}
$$

where $\hat{\epsilon}$ represents the polarization vector of the light. The matrix element can be expressed in terms of the Clebsch-Gordan coefficients and the reduced matrix element using the Wigner-Eckart theorem [11]. For the ground state of an Alkali atom ($J = 1/2$) the expression above gets simplified to

$$
\alpha^{(0)} \approx \sum_{J'} \frac{2\omega_{JJ'}|\langle J = 1/2\|\mathbf{d}\|J'\rangle|^2}{3\hbar(\omega_{JJ'}^2 - \omega^2)}.
\tag{3.6}
$$

The dipole matrix elements needed to compute the polarizability are related to the transition scattering rate via Fermi's golden rule [9, 11]

$$
\Gamma_{JJ'} = \frac{\omega_{JJ'}^2}{3\pi\epsilon_0\hbar c^3} \frac{2J+1}{2J'+1} |\langle J\|\mathbf{d}\|J'\rangle|^2,
\tag{3.7}
$$

and combining this with the expression for the intensity of the electric field $I(\mathbf{r}) =$

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[2]A rank k tensor can be represented by $2k+1$ irreducible tensor operators, which are collection of operators that transforms under rotations like the spherical harmonics $Y_{kq}(\theta, \phi)$

$2\epsilon_0 c|\mathbf{E}(\mathbf{r})|^2$ we find that the energy of the ground state manifold is shifted by

$$U(\omega, \mathbf{r}) = -\frac{\pi c^2 I(\mathbf{r})}{2} \left[\frac{2\Gamma_{\text{D1}}}{\omega_{\text{D1}}^2} \left(\frac{1}{\omega + \omega_{\text{D1}}} - \frac{1}{\omega - \omega_{\text{D1}}} \right) + \frac{2\Gamma_{\text{D2}}}{\omega_{\text{D2}}^2} \left(\frac{1}{\omega + \omega_{\text{D2}}} - \frac{1}{\omega - \omega_{\text{D2}}} \right) \right],$$
(3.8)

[TODO:add the fudge factors that give more weight to one of the transitions (both here and in Gamma)] where only the the most significant contribution from the closest transitions (the D1 and D2 lines) are included. Here $U(\mathbf{r})$ is related to the real part of the polarizability which is in fact a complex valued number. So far I have only considered the real part by assuming the excited states have an infinitely long lifetime. However, in reality the atom can spontaneously emit photons and decay. This exponential decay can be accounted for by adding an imaginary contribution to the energies $\omega_D \to \omega_D + i\Gamma_D \omega^3/\omega_D^3$ of the D1 and D2 transitions [12]. The scattering rate is related to the imaginary part of the polarizability and is given by

$$\Gamma(\omega, \mathbf{r}) = \frac{\pi c^2 I(\mathbf{r})}{2\hbar} \left[\frac{2\Gamma_{\text{D1}}\omega^3}{\omega_{\text{D1}}^6} \left(\frac{1}{\omega + \omega_{\text{D1}}} - \frac{1}{\omega - \omega_{\text{D1}}} \right)^2 + \frac{2\Gamma_{\text{D2}}\omega^3}{\omega_{\text{D2}}^6} \left(\frac{1}{\omega + \omega_{\text{D2}}} - \frac{1}{\omega - \omega_{\text{D2}}} \right)^2 \right]$$
(3.9)

The energy shift $U(\omega, \mathbf{r})$ is a conservative term and is related to dipole trapping while the scattering term $\Gamma(\omega, \mathbf{r})$ is dissipative and is important for laser cooling. In the context of engineering potentials for ultracold atoms with off-resonant light, the scattering is translated into heating because every time an atom emits a photon with angular frequency ω_L it gets a recoil momentum $\hbar\mathbf{k}_L$.

If the frequency ω satisfies the relation $\omega + \omega_{\text{D}} \gg \omega - \omega_{\text{D}}$ we can neglect the terms proportional to $1/(\omega + \omega_{\text{D}})$, an approximation typically known as the rotating wave approximation (RWA). If the RWA is valid then the frequency dependence of both the energy shifts and the scattering rates will be given by the detuning from the D1 and D2 transitions.

3.2.1.1 Optical trapping

One important application of the scalar light-shift is to create optical traps for our clouds of ultracold atoms. The use optical fields with non-uniform spatial intensity can generate traps (and anti-traps) for the atoms which experience a force proportional to the intensity gradient $F_{\text{dip}} = -\nabla U(\mathbf{r})$. [TODO: make nice figure of dipole trap]. The production of BECs in our lab relies on the use of focused Gaussian laser beams. The intensity profile of a focused Gaussian beam propagating along $\mathbf{e}_z$ is given by

$$I(x, y, z) = \frac{2P}{\pi\omega^2(z)} e^{-\frac{x^2+y^2}{\omega^2(z)}}$$
(3.10)

where P is the total power of the beam and the $1/e^2$ radius is given by $w(z) = w_0\sqrt{1 + z^2/z_R^2}$ where the minimum radius w_0 is known as the waist and $z_R = \pi\omega_0^2/\lambda$ is the Rayleigh range. If the extent of an atomic cloud is small compared to the size of the beam we can perform a Taylor expansion around $\mathbf{r} = 0$ to obtain the

trapping potential

$$U(\mathbf{r}) = -U_0 \left(1 - 2\frac{x^2 + y^2}{\omega_0^2} - \frac{z^2}{Z_R^2} \right). \tag{3.11}$$

The oscillation frequencies of the trap along the radial direction are $\omega_r = (4U_0/m\omega_0^2)^{1/2}$ and along the axial direction $\omega_z = (2U_0/mz_R)^{1/2}$. The beam waist is usually much smaller than the Rayleigh range and therefore the trap is much stronger along the axial direction. To get around this we use a 'crossed dipole trap' which is formed by a combination of two cross-polarized[3] focused Gaussian beams propagating along perpendicular axes, ensuring that we get good confinement of atoms along all spatial directions.

For a given trapping potential $U(\mathbf{r})$, the density distribution of a thermal ensamble is

$$n(\mathbf{r}) = n_0 e^{-\frac{U(\mathbf{r})}{k_B T}}. \tag{3.12}$$

The temperature T can be derived from the density distribution. For a 3D harmonic trap

$$n(\mathbf{r}) = n_0 e^{-\left(\frac{x^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2} + \frac{z^2}{2\sigma_z^2}\right)}, \tag{3.13}$$

where $\sigma_i = \omega_i^{-1}\sqrt{k_B T/m}$. Using the equipartition theorem we find that the spatial extension of the cloud and the temperature are related by

$$T = \frac{m}{k_B}\sigma_i^2\omega_i^2 \tag{3.14}$$

3.2.2 Vector polarizability

The geometry and wavelength of the Raman fields determine the natural units of the system: the single photon recoil momentum $k_{\mathrm{L}} = \sqrt{2}\pi/\lambda_{\mathrm{R}}$ and its associated recoil energy $E_{\mathrm{L}} = \hbar^2 k_{\mathrm{L}}^2/2m$, as well as the direction of the recoil momentum $\mathbf{k}_{\mathrm{L}} = k_{\mathrm{L}}\mathbf{e}_x$. The Raman wavelength was $\lambda_{\mathrm{R}} = 790.032$ nm, as usual, so that the scalar light shift is zero.

3.2.2.1 Raman induced transitions and spin-orbit coupling

[TODO: make plots of gamma, us and uv. Use data from atoms as an example?]

[Something about what we use this transitions for and how we usually ignore all other levels. (???)]

[TODO: what about matrix elements between -1 and +1?. Move to intro chapter]

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[3]The beams are cross-polarized to avoid interference between them

3.3 Magnetic interaction

3.3.1 Static magnetic fields

Also talk about the Paschen–Back effect occurs in a strong external magnetic field. The spin and orbital angular momen- tum precess independently about the magnetic field.

Uniform fields: Zeeman splitting, Breit-Rabi formula Gradients: Quadrupole potentials and Stern-Gerlach

3.3.2 Oscillatory magnetic fields

RF coupling and microwave coupling

3.4 Applications

3.4.1 Quantum coherent dynamics?

3.4.2 Adiabatic rapid pasage

3.4.3 The Rabi cycle

3.4.4 Ramsey interferometry

3.5 Floquet theory

3.6 Absorption imaging

3.6.1 Time of flight imaging

3.6.2 Partial transfer absorption imaging: magnetic field stabilization

We then apply a pair of $250\,\mu$s microwave pulses that each transfer a small fraction of atoms into the $5^2\mathrm{S}_{1/2}$ $f = 2$ manifold that we use to monitor and stabilize the bias field [13]. The microwave pulses are detuned by ± 2 kHz from the $|f = 1, m_F = 0\rangle \leftrightarrow |f = 2, m_F = 1\rangle$ transition and spaced in time by $33\,\mathrm{ms}$ (two periods of $60\,\mathrm{Hz}$). We imaged the transferred atoms following each pulse using absorption imaging[4], and count the total number of atoms n_1 and n_2 transferred by each pulse. The imbalance in these atom numbers $(n_1 - n_2)/(n_1 + n_2)$ leads to a 4 kHz wide error signal that we use both to monitor the magnetic field before each spectroscopy measurement and cancel longterm drifts in the field.

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[4]We did not apply repump light during this imaging, so the untransferred atoms in the $f = 1$ manifold were largely undisturbed by the imaging process.

3.7   Floquet

How to treat systems when RWA is not valid and how to create new effective (stroboscopic) Hamiltonians.

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