Optical trapping and manipulation of atoms near surfaces
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This chapter provides the theoretical background needed for the rest of this thesis. The first section deals with the description of light in general and evanescent waves in particular. A generalized expression for the intensity of light is derived, that can also be applied to evanescent waves. Subsequently, some equations for dealing with diffraction limited, finite-size beams are presented.

The third section focuses on the interaction of atoms with light. Special attention is paid to the description of multi-level atoms and the different conventions used in the literature. The spontaneous light pressure force and the dipole force are introduced. Accurate information of the $^{87}$Rb $D$ lines is given. The last section deals briefly with the Van der Waals interaction of atoms in the vicinity of a dielectric surface.
2.1 Propagating and evanescent light

This section focuses on the description of light fields as they occur in our experiment. The main result will be the derivation of some characteristics of evanescent waves. Since an evanescent wave is not a propagating wave and the energy flux perpendicular to the surface is imaginary, we have to modify the usual expression for the intensity. Since many of the equations dealing with the interaction of atoms with light are expressed in terms of the light intensity, they are not straightforwardly applicable to the case of atoms interacting with evanescent waves. In the first parts of this section we will deal with plane waves and an effective intensity is defined that is generally usable for describing the interaction of atoms with electromagnetic waves. Subsequently some basic concepts of evanescent waves are defined and we will introduce the concept of the evanescent-wave intensity. Finally we will focus on some effects specific for circularly-polarized evanescent waves.

2.1.1 Plane waves, definitions and refraction phenomena

We consider a plane monochromatic light wave with an electric-field component \( \mathbf{E}(x, t) \) at position \( x \) and time \( t \). It is described by

\[
\mathbf{E}(x, t) = \mathcal{R} \left( \mathbf{E}_0 e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)} \right),
\]

(2.1)

with angular frequency \( \omega \), wavevector \( \mathbf{k} \), and \( \mathbf{E} \) a complex vector describing the amplitude and the polarization of the wave. The symbol \( \mathcal{R}(\cdot) \) denotes the real part of an expression. The frequency \( \omega \) and the amplitude \( k \) of the wavevector \( \mathbf{k} \) are proportional \( k = (n/c)\omega \). Here \( c \) is the velocity of light in vacuum and \( n \) the refractive index of the medium in which the wave propagates; the fraction \( c/n \) is the velocity of light in this medium. Since we consider monochromatic light we can consider \( n \) to be constant. The wavevector \( \mathbf{k} \) is parallel to the propagation direction of the wave. The wavelength \( \lambda \) is defined by \( \lambda = 2\pi/k \). In vacuum, with \( n = 1 \), we define the free space wavevector \( k_0 = \omega/c \) and the free space wavelength \( \lambda_0 = 2\pi/k_0 \).

When this plane wave hits a boundary, separating two media with different optical properties, it will be partially reflected and partially transmitted. In this section we consider a plane wave, incident at an angle \( \theta_i \) with respect to the surface normal, as is shown in Fig. 2.1. This figure also shows the geometry in which we will describe this problem. The surface boundary is in the \( Oxy \) plane and the plane of incidence of the wave is in the \( Oxz \) plane. The angle of the reflected wave \( \theta_r \) is equal to \( \theta_i \), and the angle of the transmitted wave \( \theta_t \) is given by Snell's law

\[
\frac{\sin \theta_i}{\sin \theta_t} = \frac{n_1}{n_2}.
\]

(2.2)

The wavevector \( \mathbf{k}_i \) of the incident wave in this geometry is given by

\[
\mathbf{k}_i = n_1 k_0 \left( \sin \theta_i, 0, \cos \theta_i \right),
\]

(2.3)
2.1 Propagating and evanescent light

![Schematic representation of the geometry of a beam reflected and refracted from a surface boundary between two media with refractive indices \(n_1\) and \(n_2\). Since the refracted angle \(\theta_i\) is larger than the angle of incidence \(\theta_i\), \(n_1 > n_2\) for this example.]

and the electric-field amplitude \(\vec{E}_i\) of this wave is now

\[
\vec{E}_i = (-E_i^{TM} \cos \theta_i, E_i^{TE} e^{i\varphi}, E_i^{TM} \sin \theta_i).
\] (2.4)

Here \(E_i^{TM}\) and \(E_i^{TE}\) represent the components of the electric-field vector parallel respectively perpendicular to the plane of incidence \(Oxz\). The exponent \(\exp(i\varphi)\) describes the phase difference between the TE and TM-polarized components. Similar equations hold for the wavevector of the reflected field \(\vec{k}_r\) and the transmitted field \(\vec{k}_t\), and for the reflected electric field \(\vec{E}_r(x,t)\) and the transmitted electric field \(\vec{E}_t(x,t)\).

For these plane waves the corresponding magnetic field is given by

\[
\vec{H} = \sqrt{\frac{\varepsilon}{\mu k}} \times \vec{E},
\] (2.5)

with \(\varepsilon\) the electric, and \(\mu\) the magnetic permeability of the medium.

2.1.2 Energy density and energy flow

The time-averaged energy density \(u\) of a wave or field that obeys Maxwell’s equations is in general defined by

\[
u = \frac{1}{4} \left( \vec{E} \cdot \vec{D}^* + \vec{B} \cdot \vec{H}^* \right),
\] (2.6)

where we have introduced the electric displacement \(\vec{D} = \varepsilon\vec{E}\) and the magnetic induction \(\vec{B} = \mu\vec{H}\). Here we follow the terminology of Jackson [47]. Unless specified otherwise, we will work in S.I. units throughout this thesis. The first term is called
the time-averaged energy density of the electric field $u_E$ and the second term is the time-averaged energy density of the magnetic field $u_H$. From Eqs. (2.5) and (2.6) it is obvious that the electric and magnetic-field energy densities are equal for a plane wave. For the specific case of a plane wave, the total time-averaged energy density reduces to

$$u_{pw} = \frac{1}{2} \varepsilon |\mathbf{E}|^2,$$  \hspace{1cm} (2.7)

where the subscript “pw” denotes plane wave.

The time-averaged energy flow is in general defined by Poynting’s vector $\mathbf{S}$

$$\mathbf{S} = \frac{1}{2} \mathbf{E} \times \mathbf{H}^*,$$  \hspace{1cm} (2.8)

which for a plane wave, by substituting Eq. (2.5), reduces to

$$\mathbf{S}_{pw} = \frac{\varepsilon c}{2n} |\mathbf{E}|^2 \frac{\mathbf{k}}{k}.$$  \hspace{1cm} (2.9)

The amplitude $|\mathbf{S}_{pw}|$ is equal to the intensity $I$ of the wave and it points in the direction of propagation. This intensity $I$ can also be defined from the energy density (2.7)

$$I = u_{pw} \frac{c}{n}.$$  \hspace{1cm} (2.10)

The main reason why we are interested in the intensity of light is because we want to determine its interaction with atoms, which we will examine in more detail in section 2.3. This interaction is, however, almost completely dominated by the electric-field component of the light. For plane waves the intensity $I$ is a valid parameter to describe this interaction because the energy densities of the electric and magnetic fields are equal under all circumstances. It is commonly used because it is an experimentally convenient quantity. A more generally applicable quantity would be the electric energy density $u_E$, or the electric-field energy flux density $u_Ec/n$. Based on this we can define an effective intensity $I_{eff}$, which is generally valid for describing the interaction of atoms with light

$$I_{eff} = \frac{2c}{n} u_E = \frac{\varepsilon c}{2n} \mathbf{E} \cdot \mathbf{E}^*.$$  \hspace{1cm} (2.11)

In the remainder of this thesis we will drop the subscript “eff”. For virtually all optical materials $\mu = \mu_0$ is satisfied and the pre factor $\varepsilon c/2n$ in Eqs. (2.9) and (2.11) can be replaced by $n\varepsilon_0c/2$.

### 2.1.3 Evanescent waves

When a light wave is refracted from a medium with a higher index of refraction $n_1$ to a medium with a lower index of refraction $n_2 < n_1$, the refracted wave propagates more parallel to the surface. Using Snell’s law (2.2) we can determine a critical angle $\theta_c$

$$\theta_i = \theta_c = \arcsin \frac{n_2}{n_1},$$  \hspace{1cm} (2.12)
at which the refracted wave propagates parallel to this surface, $\theta_i = \pi/2$. For even larger angles of incidence $\theta_i$, Eq. (2.2) yields a complex value for $\theta_i$, which is associated with the appearance of an evanescent wave. In the remainder of this section and the rest of this thesis we will consider evanescent waves in vacuum, thus $n_2 = 1$, near a dielectric medium with $n_1 = n$. The general result can be obtained by replacing $n$ with $n_1/n_2$ and $k_0$ with $k_0/n_2$.

For this case with $\theta_i > \theta_c$ it is convenient to write the Fresnel equations [48, 49] as follows:

$$r_{\text{TE}} = \frac{n \cos \theta_i - i \sqrt{n^2 \sin^2 \theta_i - 1}}{n \cos \theta_i + i \sqrt{n^2 \sin^2 \theta_i - 1}}, \quad (2.13)$$

$$r_{\text{TM}} = \frac{\cos \theta_i - in \sqrt{n^2 \sin^2 \theta_i - 1}}{\cos \theta_i + in \sqrt{n^2 \sin^2 \theta_i - 1}}, \quad (2.14)$$

$$t_{\text{TE}} = \frac{2n \cos \theta_i}{n \cos \theta_i + i \sqrt{n^2 \sin^2 \theta_i - 1}}, \quad (2.15)$$

$$t_{\text{TM}} = \frac{2n \cos \theta_i}{\cos \theta_i + in \sqrt{n^2 \sin^2 \theta_i - 1}}. \quad (2.16)$$

These Fresnel equations give us the reflected amplitudes $E_r^{\text{TE}} = r_{\text{TE}} E_{i}^{\text{TE}}$ and $E_r^{\text{TM}} = r_{\text{TM}} E_{i}^{\text{TM}}$, and refracted amplitudes $E_t^{\text{TE}} = t_{\text{TE}} E_{i}^{\text{TE}}$ and $E_t^{\text{TM}} = t_{\text{TM}} E_{i}^{\text{TM}}$ of the TE and TM-polarized electric-field components, directly at the surface. They show that $|r_{\text{TE}}| = |r_{\text{TM}}| = 1$ for $\theta_i \geq \theta_c$, which is called total internal reflection. The field on the transmission side is called an evanescent wave. Although this is not a plane wave, we can derive some properties by substituting the complex value of $\theta_i$ in the plane wave results of sections 2.1.1 and 2.1.2.

For example the wavevector $k_i$ can be written similar to Eq. (2.3) with $\theta_i$ replaced by $\theta_i$. By rewriting the $\sin \theta_i$ and $\cos \theta_i$ terms with use of Eq. (2.2) this results in

$$k_i = k_0 \left( n \sin \theta_i, 0, \pm i \sqrt{n^2 \sin^2 \theta_i - 1} \right), \quad (2.17)$$

from which is obvious that the component perpendicular to the surface has become imaginary. The field

$$E_i(x, t) = \Re \left( \vec{E}_i e^{i(k_0 x - \omega t)} \right) = \Re \left( \vec{E}_i e^{-k \kappa z e^{-ik_0 n \sin \theta_i} e^{-i\omega t}} \right), \quad (2.18)$$

with $\kappa = k_0 \sqrt{n^2 \sin^2 \theta_i - 1}$, represents a non-homogeneous wave propagating along the boundary and whose amplitude varies exponentially in the direction perpendicular to the boundary. It is obvious that in this case the plus sign needs to be used in Eq. (2.17) otherwise Eq. (2.18) would diverge for $z \to \infty$. The decay length $\xi$ of this evanescent wave is given by

$$\xi = \frac{1}{\kappa} = \frac{\lambda_0}{2\pi \sqrt{n^2 \sin^2 \theta_i - 1}}. \quad (2.19)$$

This decay length is typically on the order of $\lambda_0$. 

2.1 Propagating and evanescent light
2.1.4 Effective evanescent-wave intensity

By substitution of the complex value of $\theta_i$, the electric and magnetic-field vectors $\mathbf{E}_i(x,t)$ and $\mathbf{H}_i(x,t)$ become

$$\tilde{\mathbf{E}}_i = \left(-iE^\text{TM}_i \sqrt{n^2 \sin^2 \theta_i - 1}, E^\text{TE}_i e^{i\varphi}, E^\text{TM}_i n \sin \theta_i \right). \quad (2.20)$$

$$\tilde{\mathbf{H}}_i = \frac{\varepsilon_c}{n} \left(-iE^\text{TE}_i \sqrt{n^2 \sin^2 \theta_i - 1} e^{i\varphi}, -E^\text{TM}_i, E^\text{TE}_i n \sin \theta_i e^{i\varphi} \right). \quad (2.21)$$

where $\mathbf{H}_i$ is defined analogous to $\mathbf{E}_i$ in Eq. (2.18). The fields $\mathbf{E}_i(x,t)$ and $\mathbf{H}_i(x,t)$ are still orthogonal as in the plane wave case, and they are both orthogonal to $\mathbf{k}_i$ and the total energy density $u$ is still independent of the polarization. However, the electric and magnetic energy densities $u_E$ and $u_M$ are no longer equal, and their ratio depends on the polarization. Since the $z$ component of the energy flow $\mathbf{S}$ becomes imaginary [47, 48] it is not possible to define an intensity for this evanescent wave in the usual way. However, in order to describe the interaction with atoms, an effective intensity based on Eq. (2.11) can still be defined.

We now introduce transmissivity coefficients $T^\text{TE}$ and $T^\text{TM}$ for the effective evanescent-wave intensities for the TE and TM-polarized components as

$$T^\text{TM}_\text{EW} = \frac{I^\text{TM}}{I^\text{TM}} = \frac{1}{n} \frac{|E^\text{TM}_i|^2}{|E^\text{TM}_i|^2} = \frac{1}{n} (2n^2 \sin^2 \theta_i - 1) n^2 \sin \theta_i^*_{\text{TM}}, \quad (2.22)$$

$$T^\text{TE}_\text{EW} = \frac{I^\text{TE}}{I^\text{TE}} = \frac{1}{n} \frac{|E^\text{TE}_i|^2}{|E^\text{TE}_i|^2} = \frac{1}{n} n_{\text{TE}}^*_{\text{TE}}, \quad (2.23)$$

where in the last step Eq. (2.20) and the substitutions for $E^\text{TM}_i$ and $E^\text{TE}_i$ have been used. The transmissivities have been explicitly evaluated. By substituting Eqs. (2.15) and (2.16) in Eqs. (2.22) and (2.23), these transmissivities become

$$T^\text{TM}_\text{EW} = \frac{4n \cos^2 \theta_i (2n^2 \sin^2 \theta_i - 1)}{\cos^2 \theta_i + n^2 (n^2 \sin^2 \theta_i - 1)}, \quad (2.24)$$

$$T^\text{TE}_\text{EW} = \frac{4n \cos^2 \theta_i}{n^2 - 1}. \quad (2.25)$$

2.1.5 Elliptically and circularly-polarized evanescent waves

From Eqs. (2.20) and (2.21) it is clear that a TM-polarized incident wave leads to an “elliptically-polarized” and a TE-polarized incident wave to a “linearly-polarized” electric field at the vacuum side of the surface. In the latter case, however, the magnetic field has a similar “elliptical polarization” as the electric field in the first case. The fact that the “polarizations” of the electric and magnetic fields are different is another striking difference between the evanescent and the more common propagating light fields. The aspect ratio of this elliptical polarization depends on the angle of incidence of the incident wave. In the limit of $\theta_i$ approaching the critical angle $\theta_c$, the polarization tends to linear.
2.2 Description of diffraction limited beams

With $\varphi = \pm \pi/2$ and $E_t^{\text{TE}} = E_t^{\text{TM}}$, Eq. (2.20) represents a circularly-polarized evanescent wave. The plane of polarization is however not perpendicular to the real part of the $k$ vector $\mathcal{R}(k)$ as in the case of a propagating wave. Instead it makes an angle in the $Oxy$ plane with $\mathcal{R}(k)$ of $\chi = \arctan(\sqrt{n^2 \sin^2 \theta_i - 1})$. This angle is equal to the angle between the Poynting vector and $\mathcal{R}(k)$. Fig. 2.2 shows this angle $\chi$ as a function of the angle of incidence $\theta_i$ for a medium with $n = 1.5$. For $\theta_i = \theta_c + 20$ mrad this tilt angle is $12^\circ$ and it increases up to $48^\circ$ when $\theta_i$ approaches $\pi/2$.

2.2 Description of diffraction limited beams

The description of light beams presented in the previous section is valid for plane waves. Many features of a physically realistic beam with a finite beam diameter can be properly described by a plane wave. However, this is not sufficient e.g. in the case of total internal reflection, for angles of incidence very close to the critical angle. This is important for the analysis of experiments where atoms are probed using evanescent fields, that is presented in chapter 6. In the first part of this section is derived how a diffraction limited beam can be treated as a coherent superposition of plane waves. The second part of this section describes how the reflected and transmitted fields can be calculated. Also a method to determine the effective EW intensity is presented.

2.2.1 Propagating beam equations

A plane wave propagating in the $xz$ plane at an angle $\theta$ with the $z$ axis is described by $\exp(ik_x(\theta)x)\exp(ik_z(\theta)z)$, as is obvious from Eq. (2.1), with $k_x(\theta) = nk_0 \sin \theta$ and $k_z(\theta) = nk_0 \cos \theta$. Here $n$ is the index of refraction of the medium. A Gaussian beam can be described as a coherent sum over several propagation directions $\theta$. 
These are normally distributed around a central value $\theta_0$ and the distribution has a $1/e$ width of $\phi$. From the theory of Gaussian beams [49, 50], we know that the far field divergence of a beam is equal to $\lambda_0/\pi w_0$, with $\lambda_0$ the wavelength of the light and $w_0$ the waist (minimum $1/e$ radius of the electric field distribution) of the beam. This divergence is equal to the angular spread $\phi$

$$\phi = \frac{\lambda_0}{\pi w_0}. \quad (2.26)$$

The electric field distribution of a propagating beam is now given by

$$E(x, z) = \frac{1}{\pi \phi} \int_{0}^{2\pi} e^{ik_x \phi} e^{-ik_y \phi} e^{-i\omega_0 d(\theta - \theta_0)^2/2} e^{-i(\theta - \theta_0)^2/\phi^2} d\theta, \quad (2.27)$$

where the factor $\exp(ink \theta - \theta_0)^2/2)$ displaces the waist by a distance $d$ along the propagation direction of the beam. The integral is normalized such that $|E|^2 = 1$ in the waist of the incident beam. Eq. (2.27) is completely similar to the more common notation in the literature where the integration is over the wavevector [50], instead of over the angle of the wavevector with an interface.

### 2.2.2 Reflection and transmission

The reflection of a propagating wave given by Eq. (2.27) from a boundary at $z = 0$ between a medium with index of refraction $n_1 = n$ and a medium with index of refraction $n_2 = 1$, as depicted in Fig. 2.1, is described by

$$t(\theta) = \int_{-\pi/2}^{\pi/2} t(\theta) e^{i k_x \phi} e^{-i k_y \phi} e^{-i \omega_0 d(\theta - \theta_0)^2/2} e^{-i(\theta - \theta_0)^2/\phi^2} d\theta, \quad (2.28)$$

where $r(\theta)$ is a Fresnel reflection coefficient $r_{TE}(\theta)$ or $r_{TM}(\theta)$, as defined by Eqs. (2.13) and (2.14), depending on the polarization of the light. Obviously only the vector $k_z$ has changed sign with respect to Eq. (2.27). We have restricted the angle of incidence $\theta_0$ here to $-\pi/2 < \theta_0 < \pi/2$.

The propagating part of the wave that is transmitted through this boundary is described by

$$E_t(x, z) = \frac{1}{\pi \phi} \int_{0}^{\pi/2} t(\theta) e^{i k'_{z} \phi} e^{-i k'_{y} \phi} e^{-i \omega_0 d(\theta - \theta_0)^2/2} e^{-i(\theta - \theta_0)^2/\phi^2} d\theta, \quad (2.29)$$

where $t(\theta)$ is a Fresnel transmission coefficients $t_{TE}(\theta)$ or $t_{TM}(\theta)$, as defined by Eqs. (2.15) and (2.16), depending on the polarization of the light. The wavevectors $k'_{z}$ and $k'_{y}$ are defined by $k'_{z} = n k_0 \sin \theta$ and $k'_{y} = k_0 \sqrt{1 - n^2 \sin^2 \theta}$. The evanescent part of the transmitted field is described by

$$E_{EW}(x, z) = \frac{1}{\pi \phi} \int_{\pi/2}^{\pi/2} t(\theta) e^{i k'_{z} \phi} e^{-z/\xi(\theta)} e^{-i \omega_0 d(\theta - \theta_0)^2/2} e^{-i(\theta - \theta_0)^2/\phi^2} d\theta, \quad (2.30)$$

where the decay length $\xi(\theta)$ is defined by Eq. (2.19).
In order to calculate the effective intensity of the evanescent field one needs to take care of the extra pre factors of Eqs. (2.22) and (2.23). This is done by replacing the Fresnel transmission coefficient \( t(\theta) \) by the square root of the corresponding evanescent-wave transmissivity \( \sqrt{T_{EW}(\theta)} \), as defined by Eqs. (2.24) and (2.25). The absolute value of the square of the resulting integral scales with the intensity. Due to the special normalization of Eq. (2.27), the EW intensity distribution is now given by

\[
I_{EW}(x, z) = I_1 \left| \frac{1}{\pi \theta} \int_{\theta_e}^{\pi/2} \sqrt{T_{EW}(\theta)} e^{i k z(\theta)} e^{-z \xi(\theta)} e^{-i k_0 d(\theta-\theta_0)^2/\phi^2} d\theta \right|^2,
\]

with \( I_1 \) the maximum intensity of the incident beam at the boundary.

## 2.3 Atoms and their interaction with light

In this section we describe the interaction of atoms with monochromatic light. We will focus mainly on mechanical effects on the atom. In the first part we will describe the hypothetical situation of a two-level atom to demonstrate the two different forces acting on an atom. In the second part we will extend this to multi-level atoms and finally we will apply it to the case of \(^{87}\text{Rb}\) atoms.

### 2.3.1 Two-level atoms

For a two-level atom with a resonance frequency \( \omega_0 \) we denote the ground state by \( |g\rangle \) and the excited state by \( |e\rangle \). The excited state has a lifetime \( \tau = 1/\Gamma \), where \( \Gamma \) is the the decay rate or the linewidth of the transition.

When this atom interacts with a light field with frequency \( \omega \) and intensity \( I \), two physically different contributions of the force acting on the atoms can be distinguished. A force associated with the scattering (absorption and spontaneous emission) of photons, and a force associated with the interaction of the electric field of the light with the electric dipole that is induced in the atom. A beautiful derivation of these two forces is shown in [51] section V.C.2. In the following discussion we will, however, follow a more intuitive approach.

**Near resonance effects I - spontaneous light pressure force** This effect is particularly important for relatively small detunings, \( \delta = \omega - \omega_0 \). The process of absorption of a photon from the light field and spontaneously emitting it in another mode is then the dominant process.

The atom receives a momentum kick of \( \hbar k \) for every absorbed photon. A subsequent stimulated emission process results in a momentum change \( -\hbar k_{\text{out}} \). Due to the random character of a spontaneous emission process, the momentum change due to this process averages out over many absorption-emission cycles and only results in heating. This yields a net momentum change of \( \hbar k \) per cycle. The average force
encountered by the atom, which is called the *spontaneous light pressure force*, is thus

\[ F_{sp} = \hbar k \Gamma'. \] (2.32)

with \( \Gamma' \) the scattering rate, which is the product of the excited state population and the decay rate \( \Gamma \). For a constant intensity the scattering rate tends to a steady state value

\[ \Gamma' = \frac{\Gamma}{2} \frac{s}{s + 1}. \] (2.33)

here \( s \) is the so called saturation parameter

\[ s = \frac{1}{1 + \left( \frac{\delta}{\Gamma} \right)^2 I_0}, \] (2.34)

with

\[ I_0 = \hbar \omega^3/12\pi c^2 \] (2.35)

the saturation intensity of the transition.

**Near resonance effects II - Doppler cooling** For a moving atom the effective detuning of the light beams depends on the velocity \( \mathbf{v} \) of the atoms due to the Doppler shift \( \delta_D = -\mathbf{k} \cdot \mathbf{v} \). For two counterpropagating laser beams, with wavevectors \( \pm \mathbf{k} \) and equal detuning \( \delta \), the interaction of a moving atom with the beams is different due to the difference in Doppler shift. Naturally the direction of the radiation pressure is in opposite directions. The net force acting on the atom is now

\[ \mathbf{F}_D = (\mathbf{F}_{sp})_{\delta - \delta - \mathbf{k} \cdot \mathbf{v}} - (\mathbf{F}_{sp})_{\delta - \delta + \mathbf{k} \cdot \mathbf{v}}. \] (2.36)

with \( \mathbf{F}_{sp} \) defined by Eq. (2.32)-(2.35). The subscripts \( \delta \rightarrow \delta \pm \mathbf{k} \cdot \mathbf{v} \) denote that the Doppler shift needs to be incorporated in the detuning in Eq. (2.34). For small saturation, such that \( \Gamma' \approx s \Gamma/2 \) and \( |\mathbf{v}| \ll |\delta|/k_0 \) this force is approximated, to second order in \( |\mathbf{v}| \), by

\[ \mathbf{F}_D = 8 \hbar k_0^2 I_0 \Gamma \frac{\mathbf{v}}{\left( 1 + \left( \frac{\delta}{\Gamma} \right)^2 \right)^2} \approx -\beta \mathbf{v}. \] (2.37)

For small red detunings \( \delta \approx -\Gamma/2 \) and small atomic velocities \( |\mathbf{v}| \) this force is a substantial damping force resulting in cooling of the atom, which is called *Doppler cooling*. The lower bound of the temperature is determined by the random nature of the spontaneous emission process. This lowest reachable temperature is the Doppler temperature \( T_D = \hbar \Gamma/2k_B \), with \( k_B \) Boltzmann’s constant.

**Far off-resonance effects - dipole force** For large detunings \( |\delta| \gg \Gamma \), the off-resonant driving of the atom induces a dipole \( \mathbf{d} = \alpha \mathbf{E} \) in the atom, with \( \alpha \) the polarizability of the atom. When \( |\delta| \gg \Omega_R \), with \( \Omega_R = \mathbf{d} \cdot \mathbf{E}/\hbar \) the Rabi frequency, and \( \hbar \) Plank’s constant, the spontaneous light pressure force is no longer
the dominant force that acts on the atom. The time-averaged potential energy of the induced dipole $\mathbf{d}$ in the applied field $\mathbf{E}$ is called the light shift and is given by

$$U_{\text{dip}} = -\frac{1}{2}\langle \mathbf{d} \cdot \mathbf{E} \rangle = -\frac{1}{4}\alpha|\mathbf{E}|^2 \approx \frac{\hbar s\delta}{2}.$$ (2.38)

where $\langle \cdot \rangle$ denotes taking the time average over an optical period, and $\mathbf{E}$ is the electric field as defined in Eq. (2.1). When the transition is driven above (below) the resonance frequency $\omega$, the polarizability $\alpha$ is negative (positive), and thus the resulting potential is repulsive (attractive). Such a light field with $\delta > 0$ ($\delta < 0$) is called blue detuned (red detuned). The dipole force acting on the atom is now given by $\mathbf{F}_{\text{dip}} = -\nabla U_{\text{dip}}$. The scattering rate in the limit of large detunings and low saturation is given by

$$\Gamma' = \frac{s\Gamma}{2}.$$ (2.39)

From the ratio of the scattering rate $\Gamma'$ and the light shift $U_{\text{dip}}$

$$\frac{\hbar \Gamma'}{U_{\text{dip}}} = \frac{\Gamma}{\delta},$$ (2.40)

it is clear that for a large detuning $\delta$ and a sufficiently large intensity, so that the light shift $U_{\text{dip}}$ remains constant, the scattering rate becomes negligibly small, and the potential $U_{\text{dip}}$ becomes conservative.

### 2.3.2 Multi-level atoms

The results of the previous section are generalized to the case of realistic multi-level atoms. First, the formalism which is used to describe these atoms and the transitions between different levels is explained. Subsequently, the results for small detunings are briefly described. The effects for large detunings will be treated somewhat more extensively because of their importance for the remainder of this thesis.

**Formalism** In realistic, multi-level atoms, transitions between different states have different probabilities or transition strengths. The transition strength of the transition between the initial state $|F'm_q\rangle$ and the final state $|F'm_q'\rangle$ is described by its dipole matrix element $\langle F'm'|\mathbf{D}|F'm\rangle$, with $\mathbf{D} = e\mathbf{x}$ the dipole operator. $F$ and $F'$ are the total angular momentum quantum numbers of this initial and final state respectively, and $m$ and $m'$ are the magnetic quantum numbers of the initial and final magnetic sub-states respectively. Using the Wigner-Eckart theorem [52, 53, 54], this element can be written as

$$\langle F'm'|\mathbf{D}|F'm\rangle = \langle F'|\mathbf{D}|F\rangle \langle Fm1q|F'm'\rangle,$$ (2.41)

where the first factor is the reduced dipole matrix element, which is independent of the level sub-structure and of the polarization of the light, and the second factor is a Clebsch-Gordan coefficient, which describes the coupling between the magnetic sub-levels for a particular polarization of the light.
It will turn out to be convenient to project the polarization \( \mathbf{e} = \mathbf{E}/|\mathbf{E}| \) of the light on a coordinate system of spherical polarizations \( \epsilon_q \) with \( q = -1, 0, +1 \) denoting \( \sigma^- \), \( \pi \) and \( \sigma^+ \)-polarized light respectively, all with respect to a chosen quantization axis. The subscript \( q \) is the same that appears in the Clebsch-Gordan coefficient of Eq. (2.41).

We have to be aware of the fact that many textbooks on quantum theory of angular momentum [52, 53, 54] use an alternative definition of the reduced dipole matrix which is \( \sqrt{2F'+1} \) times larger. One can distinguish between the two definitions by examining the notation of the Wigner-Eckart theorem. To reduce confusion, throughout this thesis we will denote this alternative definition with parentheses \((\cdot | \cdot || \cdot)\) instead of angular brackets \( \langle | \cdot || \cdot \rangle \). This alternative definition is sometimes convenient since it satisfies \((F'||\mathbf{D}||F) = (F||\mathbf{D}||F')\) and it will therefore be used in the next chapter. Moreover the notation in most textbooks is chosen such that it most straightforwardly describes emission processes, which is convenient for spectroscopic purposes.

The reduced dipole matrix element can be further simplified by applying the expression [52, 53, 54]
\[
\langle F'||\mathbf{D}||F \rangle = d_{FF'} \langle J'||\mathbf{D}||J \rangle,
\]
(2.42)
where \( J \) and \( J' \) are total electronic angular momentum quantum numbers, and
\[
d_{FF'} = (-1)^{F+J'+1} \sqrt{(2J'+1)(2F+1)} \begin{pmatrix} F & F' & 1 \\ J' & J & I \end{pmatrix} \}_{6j}.
\]
(2.43)
Here \( \{\ldots\}_{6j} \) denotes the Racah 6j symbol, and \( I \) is the nuclear spin. The reduced dipole matrix for \( J \) can, analogously, be further simplified by applying
\[
\langle J'||\mathbf{D}||J \rangle = d_{JJ'} \langle L'||\mathbf{D}||L \rangle,
\]
(2.44)
where \( L \) and \( L' \) are orbital angular momentum quantum numbers, and
\[
d_{JJ'} = (-1)^{J+L+S+1} \sqrt{(2L'+1)(2J+1)} \begin{pmatrix} J & J' & 1 \\ L' & L & S \end{pmatrix} \}_{6j},
\]
(2.45)
with \( S \) the intrinsic electronic spin quantum number.

**Special case - alkali atoms** For the \( D_1 \) and \( D_2 \) lines of alkali atoms we will use subscripts \( g \) and \( e \) for the ground-state and excited-state properties, respectively. The factor \(|d_{L_e L_e}| = 1\), since \( L_g = 0, L_e = 1 \), and \( S = \frac{1}{2} \). For the transition from the \( F_g = F_{g,\text{max}} = L_g + S + I = \frac{3}{2} + I \) ground-state hyperfine level to the \( F_e = F_{e,\text{max}} = L_e + S + I = \frac{3}{2} + I \) excited state hyperfine level of the \( D_2 \) line, the value for \(|d_{F_g F_e}| = 1\), for every integer and half-integer value of \( I \). Furthermore, for every integer and half-integer value of \( F_g \), the Clebsch-Gordan coefficient \( \langle F_g, \pm m_g, 1, q = \pm 1 | F_e = F_g + 1, m_e = \pm (m_g + 1) \rangle = 1 \). By combining the above information with Eqs. (2.41)-(2.45) we can deduce
\[
|\langle F_{e,\text{max}}, m_{F_e} = \pm F_{e,\text{max}} | \mathbf{D} | F_{g,\text{max}}, m_{F_g} = \pm F_{g,\text{max}} \rangle| = |\langle L_e = 1 | \mathbf{D} | L_g = 0 \rangle|.
\]
Since this is a closed transition the value of this matrix element equals the value of the dipole moment $D$ of a two-level transition

$$ D = |\langle F_{e,\text{max}}, m_e = \pm F_{e,\text{max}} | \hat{D} | F_{g,\text{max}}, m_g = \pm F_{g,\text{max}} \rangle| = \sqrt{\frac{3\pi\varepsilon_0 c^3 \hbar \Gamma}{\omega_0^3}}. \quad (2.46) $$

Using Eq. (2.46), Eqs. (2.41)-(2.45) can be simplified to

$$ \langle F_{g,m_F} | \hat{D} | F_{e,m_F} \rangle = \langle F_{e,m_F} | \hat{D} | F_{g,m_F} \rangle = D d_{F_F} \langle F_{g,m_g} | q | F_{e,m_e} \rangle. \quad (2.47) $$

This expression is valid for all transitions of the alkali $D$ lines.

**Near resonance effects**  Near-resonant phenomena like laser cooling in multi-level atoms results in effects like polarization-gradient cooling and velocity selective coherent population trapping (VSCPT). For a description of these effects we refer to [55]. The Doppler temperature $T_D$ is no longer the lower bound for the obtainable temperatures. The new lower boundary for polarization-gradient cooling is the recoil temperature $T_r$ which is the temperature associated with the kinetic energy due to the recoil of one photon, while with VSCPT even lower temperatures can be reached. In practice atomic density induced effects like photon re-absorption will also limit the achievable temperatures.

**Far off-resonance effects** In order to calculate the light shift of a certain level $|Fm\rangle$, the contributions of the coupling to the various intermediate states $|F'm\rangle$ to the polarizability must be taken into account. Furthermore due to the substructure of the state $F$, the polarizability $\alpha$, introduced as a scalar for two-level atoms, has to be described by a tensor $\alpha$. Its indices are the initial and final magnetic substates $m$ and $m''$ and the polarizations $q$ and $q'$ of the absorbed and emitted photons, necessary to make the Raman transition.

In the case of low saturation and large detuning from resonance $|\delta_{FP'}| \gg \Gamma$, so that spontaneous emission processes can be neglected, we can derive an expression for the polarizability tensor, using time dependent perturbation theory

$$ \alpha = \sum_{F'',m''} \frac{\langle F'm'' | \hat{D} | F'm' \rangle \langle F'm' | \hat{D} | Fm \rangle}{\hbar \delta_{FP}}. \quad (2.48) $$

where $\delta_{FP}$ denotes the detuning of the light with respect to the transition frequency $\omega_{PP'}$ between the initial state $|F\rangle$ and the intermediate state $|F'\rangle$. We have assumed $\delta_{FP} \ll \omega_{PP'}$, so that the rotating wave approximation can be applied. The light shift operator $U_{\text{dip}}$ is written analogously to Eq. (2.38) as

$$ U_{\text{dip}} = -\frac{1}{2} \langle \mathbf{E}^\ast \cdot \alpha \cdot \mathbf{E} \rangle = -\frac{1}{4} \tilde{\mathbf{E}}^\ast \cdot \alpha \cdot \tilde{\mathbf{E}}, \quad (2.49) $$

where the contractions are over the polarization states of the photons, and $\langle \cdot \rangle$ again denotes averaging over an optical period. $U_{\text{dip}}$ is a tensor whose indices are the
initial and final magnetic substates $m$ and $m''$. Its eigenvalues are the light shifts of the various magnetic sub-levels of state $F$.

When the frequency of the applied optical field is much closer to the $D$ lines than to other transitions in the spectrum, only the coupling to the $D$ lines needs to be considered. This significantly simplifies the calculation. Combining Eqs. (2.49) and (2.48), while substituting Eq. (2.47) yields

$$U_{F_k} = \frac{\hbar}{8} \sum_{F_k,m_e} \frac{d^2_{F_k,F_e}}{\delta_{F_k,F_e}} \left( \epsilon^* \cdot \langle F_k m_g 1 q | F_e m_e \rangle \langle F_g m_g 1 q | F_e m_e \rangle \cdot \epsilon \right).$$

(2.50)

where the intensity $I$, the saturation intensity $I_0$, and the dipole $D$ are used, as defined in Eqs. (2.9), (2.35), and (2.47) respectively. Again the notation $\epsilon = \mathbf{E}/|\mathbf{E}|$ is used for the polarization of light.

### 2.3.3 Rubidium

The element Rb has two naturally occurring isotopes. The $^{85}$Rb isotope is a stable isotope with a natural abundance of 72.17% [56]. The $^{87}$Rb isotope has a nuclear lifetime of $4.88 \times 10^{10}$ yr [56], making it a stable isotope for all our purposes. It has a natural abundance of 27.83(2)% [56]. For atomic physics experiments aiming at quantum degeneracy $^{87}$Rb is the favorite isotope due to its favorable collisional properties.

All experiments described in this thesis are performed with $^{87}$Rb atoms. The useful transitions are the $D_1$ line around $\lambda_0 = 795.0$ nm and the $D_2$ line around $\lambda_0 = 780.2$ nm. The energy levels, including the hyperfine splittings of these transitions, are shown in Fig. 2.3. Fig. 2.4 shows the relative transition strengths $d^2_{F_k,F_e} \langle F_g m_g 1 q | F_e m_e \rangle^2$ between all the magnetic sub-levels of the $D_1$ and the $D_2$ lines. According to Eq. (2.46), the transition dipole moment $D$ in Eq. (2.47) is $D = 2.534(3) \times 10^{-29}$ Cm.

In Table 2.1 some general information of Rb is presented. In many instances the closed $|2, \pm 2 \rangle \rightarrow |3, \pm 3 \rangle$ transition of the $D_2$ line can be considered as an effective two-level system. Some parameters associated with laser cooling are also given for this transition. An extensive overview of Rb parameters is presented by Steck [57].

### 2.4 Van der Waals interaction

The experiments described in this thesis will all involve atoms in close proximity of a dielectric surface. At these small distances the Van der Waals potential has to be taken into account. The Van der Waals potential for an atom in vacuum at a distance $z$ from a flat medium with index of refraction $n$ is given by

$$U_{vdW} = -\frac{n^2 - 1}{n^2 + 1} \frac{\mathcal{D}^2}{148\pi \varepsilon_0 z^3},$$

(2.51)

which is derived in [58], Eq. (37). The factor $\mathcal{D}^2$ is the variance of the atomic electric dipole in the atomic state under consideration. Eq. (2.51) is only valid if
this state has no quadrupolar component. An expression for \( D^2 \) is derived in [58] section III.A.3. By using this expression the quantum mechanical expression Eq. (2.51) approaches the common expression for the Van der Waals potential, which is given by

\[
U_{vdW} = -\frac{3}{16} \frac{n^2 - 1}{n^2 + 1} \left( \frac{1}{k_0 z} \right)^3 \hbar \Gamma,
\]

(2.52)

to approximately 10%. For \( k_0 \) and \( \Gamma \) the values of the dominant \( D_2 \) transition of Rb atoms should be used. The experiments in [59, 60] show that this is a good approximation.

<table>
<thead>
<tr>
<th>general information on ( ^{87}\text{Rb} )</th>
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<tbody>
<tr>
<td>mass ( m = )</td>
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<td>natural abundance</td>
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<td>nuclear spin ( I )</td>
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<tr>
<th>general parameters ( D_1 ) line ( 5s^2S_{1/2} \rightarrow 5p^2P_{1/2} )</th>
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<tbody>
<tr>
<td>optical frequency ( \omega )</td>
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<tr>
<td>wavelength in vacuum ( \lambda_0 )</td>
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<tr>
<td>natural lifetime ( \tau )</td>
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<td>natural linewidth ( \Gamma/2\pi )</td>
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<td>saturation intensity ( I_0 )</td>
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<tr>
<th>general parameters ( D_2 ) line ( 5s^2S_{1/2} \rightarrow 5p^2P_{3/2} )</th>
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<tr>
<td>optical frequency ( \omega )</td>
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<td>wavelength in vacuum ( \lambda_0 )</td>
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<td>Dipole moment (</td>
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<th>Laser cooling parameters ( D_2 ) line</th>
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<tr>
<td>Doppler temperature ( T_D )</td>
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<tr>
<td>recoil temperature ( T_r )</td>
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<td>recoil velocity ( v_r )</td>
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**Table 2.1:** Some parameters of \( ^{87}\text{Rb} \).
Figure 2.3: The hyperfine levels of the $D_1$ and $D_2$ line of $^{87}$Rb. Indicated are the splittings between the several (hyper)fine-structure levels. The fine-structure splitting of the $D_1$ and $D_2$ lines is from [61] and [62] respectively. The corresponding wavelengths are calculated from these values using $\lambda_0 = 2\pi c/\omega$. The lifetimes $\tau$ of the $5p^2P_{1/2}$ and $5p^2P_{3/2}$ excited states are from [63], and the corresponding decay rates are calculated from these values by $\Gamma = 1/\tau$. The ground state hyperfine splittings are from [64] and the $5p^2P_{1/2}$ and $5p^2P_{3/2}$ excited state hyperfine splittings are from [65] and [62] respectively.
2.4 Van der Waals interaction

Figure 2.4: Relative transition strengths \(60d_{F_eF_g}^2|F_e m_{F_e} F_g, 1q|F_e m_{F_e}, F_g, 2|F_e m_{F_e}, F_g, 2|^2\) for transitions between all magnetic sub-levels of the \(D_1\) and the \(D_2\) lines.