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Diffraction of atoms by a standing-wave light field

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The University of Arizona, 1992
DIFFRACTION OF ATOMS
BY A STANDING-WAVE LIGHT FIELD

by
Erik Schumacher

A Dissertation Submitted to the Faculty of the
COMMITTEE ON OPTICAL SCIENCES (GRADUATE)
in Partial Fulfillment of the Requirements
for the Degree of
DOCTOR OF PHILOSOPHY
in the Graduate College
THE UNIVERSITY OF ARIZONA

1992
As members of the Final Examination Committee, we certify that we have read the dissertation prepared by Erik Schumacher entitled DIFFRACATION OF ATOMS BY A STANDING-WAVE LIGHT FIELD and recommend that it be accepted as fulfilling the dissertation requirement for the Degree of Doctor of Philosophy.

Pierre Meystre  2/14/92
Murray Sargent III  2/14/92
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Final approval and acceptance of this dissertation is contingent upon the candidate's submission of the final copy of the dissertation to the Graduate College.

I hereby certify that I have read this dissertation prepared under my direction and recommend that it be accepted as fulfilling the dissertation requirement.

Dissertation Director  Pierre Meystre  2/14/92
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ACKNOWLEDGMENTS

I very much enjoyed my time at the University of Arizona and the work on this dissertation, and I would like to express my thanks to all the people who made my "stay in the desert" such a valuable and great experience.

Most importantly I thank Pierre Meystre for giving me the opportunity to work in his group. He provided me with excellent guidance, motivation and support, and his physical intuition strikes me today as much as it did three years ago. As my advisor he gave me the personal freedom I needed, which allowed me to keep other interests alive.

Special thanks are due to Martin Wilkens. Not only did he provide me with many ideas and guidance for my dissertation, but he also helped me getting over the hurdles of frustration that I was subjected to in the course of this work. I benefited greatly from our teamwork, and I will certainly miss our discussions and Martin's sharp intellect in the future.

Thanks are also due to Ewan M. Wright who at times was actively involved in my research, and to M. Sargent III who made both as a physicist and computer expert a lasting impression on me. His great personality made me always feel good to be a theoretician.

I would like to express my gratitude towards the Federation of German-American Clubs and the Fulbright Commission. Their scholarships enabled me to make the leap from Germany to the University of Arizona, and thereby set the stage for this dissertation.

My parents provided me during all those years with love and support, and they were always there for me. I am especially thankful to them, since they had probably a much more difficult time than I to cope with the spatial distance that separated us.

Finally, I would like to thank Martina for all the love, joy and support she gave me during the last years.
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ABSTRACT

We study theoretically the diffraction of atoms by a standing-wave light field. Conceptually the text is divided into two parts:

In the first part we deal with the coherent interaction only. We use a band theoretical approach to describe the laser-atom interaction, and to characterize two-beam resonances (Dopplerons and Bragg resonances). These two-beam resonances are major candidates to develop effective atom beam splitters. We study the interaction with classical light fields as well as with quantum fields.

In the second part we take incoherent processes, i.e. spontaneous emission, into account and present a numerical scheme for the solution of the generalized optical Bloch equations. This scheme is based on the split-operator technique, and we use it to study numerically the influence of spontaneous emission on the diffraction process. We compare our results with recent experimental data, and investigate the impact of spontaneous emission on the performance of two-beam resonances.
CHAPTER 1

INTRODUCTION

In this thesis we theoretically investigate the diffraction of an atomic beam by a light grating. For the experiment under consideration, the roles which electromagnetic waves and matter typically play in optical diffraction experiments are interchanged. Instead of looking at the diffraction of a light beam by a mechanical grating, we study the diffraction of atomic matter-waves at the periodic potential of a standing-wave light field. The light wave effectively acts as a "light-crystal", in correspondence to the "real" crystals which have been used in x-ray, electron and neutron diffraction experiments.

In his fundamental "Treatise on Electricity and Magnetism" (1873) Maxwell was the first to point out that an electromagnetic wave propagating in a medium will exert a pressure in the direction of propagation, at each point equal to its local energy density [1]. This radiation pressure was observed experimentally in 1901 by Lebedev in Russia [2] and in 1903 by Nichols and Hull in the United States [3].

Deeper insight into the interaction between atoms and radiation, and in particular into the mechanical effects of light, was provided by quantum mechanics. Einstein discussed
in 1917 in his quantum theory of radiation the momentum transfer to molecules due to absorption and emission processes [4]. According to Bohr's quantum theory of atomic spectra, atoms absorb and emit radiation only with precisely defined energies, and Einstein concluded that the corresponding momentum transfer must also be quantized. This discrete momentum transfer from light waves to atoms was experimentally demonstrated by Frisch in 1933 [5]. He observed the deflection of a beam of sodium atoms by the resonant radiation of a sodium-pressure lamp.

Full understanding of the interaction of radiation with matter was gained in the mid-20's after de Broglie introduced "matter-waves" [6], and Schrödinger developed wave-mechanics [7]. From then on it was no longer adequate to simply treat radiation as a wave and matter as a particle, but it was evident that both matter and radiation possess a dual nature. However, while the corpuscular nature of light was demonstrated early with the photo-electric and Compton effects, the ultimate proof of the wave character of matter, namely interferences of matter-waves, needed longer to be experimentally verified. Diffraction of these matter-waves at suitable double slits or gratings was the basic idea, while an interferometer, which would use diffraction effects to first separate a (coherent) "matter-wave" beam and then recombine it again was the more sophisticated one.

Matter-wave diffraction experiments were first performed by Davisson and Germer in 1927 with electrons [8]. In 1930 Esterman and Stern reported the first diffraction experiments with molecules [9]. For these and later diffraction experiments with neutrons, crystals served as gratings.
Interferences between well separated, coherent beams with small wavelength were more difficult to demonstrate. It took until 1965 for the first interference experiments with wavelengths in the angstrom regime to be reported by Bonse and Hart [10]. They constructed an x-ray interferometer in which the beam was spatially well separated and subsequently recombined. Similar experiments were demonstrated in the 70’s with neutrons (for a review see [11]).

Further pushing the matter-wave duality, Kapitza and Dirac suggested in 1933 the diffraction of a beam of electrons at a standing-wave light field [12] based on stimulated Compton scattering. However, since the light sources available would only lead to the diffraction of a tiny part of the incoming electrons, Kapitza and Dirac concluded that the experiment would not be feasible at that time. The experiment was successfully carried out in 1965 by Bartell et al. [13].

The invention of the gas laser in the 60’s lead to renewed interest in the mechanical effects of light. The first issue was to develop a better laser theory by taking into account the ponderomotive forces exerted by the laser light on the gas molecules [14, 15]. But soon a general interest in light mechanics emerged, since the availability of light sources of high intensity, monochromaticity and directivity made it finally practicable to control atomic motion with light.

One area that rapidly gained attention was the localization and channelling of atoms by standing light waves, which Letokhov proposed in 1968 [16], and the laser cooling of atoms suggested by T. Hänsch and A. Schawlow in 1975 [17]. Later proposals suggested not only
cooling but also, e.g., the trapping of cooled atoms in a three dimensional standing light field [18]. Experiments were soon under way, and research is still very active in this field (for a recent summary see [19]).

Atomic diffraction experiments with a standing wave light field acting as a grating similar to the Kapitza-Dirac proposal for electrons were suggested first by Altshuler et al. in 1966 [20] and Ashkins in 1970 [21]. Several groups successfully reported simple experiments in the 70's [22, 23, 24, 25]. However, it took until the mid 80's for experimentalists to succeed in implementing sophisticated diffraction experiments with high momentum resolution [26, 27, 28, 27, 29, 30, 31, 32]. These experiments, performed by Pritchard et al. at MIT, demonstrated the splitting of atomic beams during the interaction, thus making atomic interferometers in principle possible. Recently the first such interference experiments were demonstrated by Carnal and Mlynek [33], Keith et al. [34], Riehle et al. [35] and Kasevitch and Chu [36].

Ultra-sensitive gravitation measurements are one area of potential usefulness for “matter-wave” interferometers. Using atoms rather than neutrons (see ref. [11]) provides for a larger sensitivity, since the de Broglie wavelength of atoms is smaller. Furthermore, an atomic beam is much easier to generate than a neutron beam. On the other hand, the interaction between atoms and light fields is quite different from the interaction between neutrons and crystals, leading to several peculiarities. The dipole moment of atoms, for example, is an induced dipole moment in contrast to the static dipole moment of neutrons. Also, the coupling of the atom to all modes of the electromagnetic field leads to spontaneous emission,
which has no equivalent in the neutron-crystal interaction.

In the following chapters we discuss atomic diffraction at a standing-wave laser field. After defining our model at the beginning of chapter 2, we introduce a band theoretical description of the coherent interaction between a standing-wave light field and an atom. Subsequently we use this band-theoretical approach to calculate the conditions for "two-beam resonances" (Bragg and Doppleron resonances) equivalent to the Bragg resonances of solid state physics. We then extend our theory to quantum fields, and investigate the effects that various initial fields have on the diffraction process, and in particular on the two-beam resonances. We illustrate all effects with computer simulations.

In chapter 3 we add to our model the effects of spontaneous emission. We present a numerical method which allows the simulation of the diffraction process in the presence of spontaneous emission, and we investigate the effects of this incoherent mechanism in various regimes. Again, numerous results from computer simulations are shown.

Our discussion ends with the conclusion in chapter 4. Three appendices give more detailed answers to the derivation of the atom-reservoir master equation, the numerical procedure, and the resonance conditions for the "two-beam" resonances. The main references are listed in the back.
CHAPTER 2

COHERENT INTERACTION

2.1 The Model

Figure 2.1 shows the experimental setup for our model. A highly collimated atomic beam traveling predominantly in the $y$-direction impinges with near normal angle of incidence on a standing-wave laser field aligned in the $x$-direction. Inside the laser beam, the atoms coherently exchange energy and momentum with the laser field. They also undergo spontaneous emission, but this incoherent process is neglected in this chapter. It will be added in chapter 3.

After leaving the laser beam, the atoms travel freely until they are detected. The detector is assumed to be sensitive to the translational state of the atom in the $x$-direction, but not to its electronic state. It is located far behind the laser, so that the momentum distribution of the outgoing atoms is measured (corresponding to Fraunhofer diffraction in classical optics).

In a frame moving at the initial speed of the atoms in the $y$-direction, the coherent
atom-laser interaction is described in the dipole- and rotating-wave approximations by the Hamiltonian [37]

\[
H = \frac{\hat{p}^2}{2M} - \hbar \delta |e\rangle \langle e| + \hbar R f(t) \cos qx (\sigma_+ + \sigma_-). \tag{2.1}
\]

Here \(\hat{p}\) is the \(x\)-component of the center-of-mass momentum of the atom, \(\hat{x}\) is the canonically conjugate position operator, \(|e\rangle\) and \(|g\rangle\) denote its excited and ground electronic state, respectively, and \(\sigma_{\pm}\) are the usual raising and lowering pseudo-spin operators; \(\delta = \Omega - \omega\) is the detuning between the laser frequency \(\Omega\) and the atomic transition frequency \(\omega\), \(q = \Omega / c\) is the wave number of the laser field, \(R = E_0 \varphi / \hbar\) is the (bare) Rabi frequency, where \(\varphi\) is the dipole moment of the transition, and \(E_0\) is half the peak amplitude of the electric field of the laser. The velocity of the incoming atoms, in combination with the diameter of the laser beam define an interaction time \(\tau\) which in turn defines the width of the laser-beam
profile function $f(t)$. For our study we will use the rectangular beam profile function

$$f(t) = \begin{cases} 
1 & \text{for } 0 < t \leq \tau, \\
0 & \text{else} \end{cases} \quad (2.2)$$

It will often prove to be convenient, to scale variables to parameters corresponding to the recoil energy, e.g. the recoil frequency $\omega_{\text{rec}} = \hbar q^2/2M$ or the recoil energy $E_{\text{rec}} = \hbar^2 q^2/2M$. The recoil energy $E_{\text{rec}}$ is the change in kinetic energy of an atom, when it exchanges a photon with a electromagnetic field with wave number $q$ and $\omega_{\text{rec}}$ is the corresponding frequency. Especially experimental parameters used for simulations will be given in these scaled units.

2.1.1 The Raman-Nath Regime

In the late 70's and early 80's the Hamiltonian (2.1) with the beam profile (2.2) has been investigated by several groups [38, 37, 39]. They paid particular attention to the regime in which the kinetic energy term $p^2/2M$ of the Hamiltonian (2.1) can be neglected, the Raman-Nath regime. In this regime the time-dependent Schrödinger equation reads

$$i\hbar \dot{\psi}(t) = [-\hbar \delta |e| + \hbar R f(t) \cos q\hat{z} (\sigma_+ + \sigma_-)]\psi(t), \quad (2.3)$$

and can be solved exactly if the initial atomic momentum is given by a $\delta$-function, and if the detuning $\delta$ is such that either $\delta \ll R$ or $\delta \gg R$ [32].
To derive the solution, we use the momentum representation, in which the wave function \( |\psi(p, t)\rangle \), is expressed by

\[
|\psi(p, t)\rangle = \langle p|\psi(t)\rangle = e(p, t)|e\rangle + g(p, t)|g\rangle,
\]

where \( e(p, t) \) and \( g(p, t) \) are the probability amplitudes for the atom at time \( t \) as a function of the momentum \( p \) for the excited state and ground state, respectively. After suitable projection, the Schrödinger equation (2.3) reads

\[
i\hbar \dot{e}(p, t) = -\hbar \delta e(p, t) + \frac{\hbar \mathcal{R}}{2} [g(p + \hbar q, t) + g(p - \hbar q, t)]
\]

\[
i\hbar \dot{g}(p, t) = \frac{\hbar \mathcal{R}}{2} [e(p + \hbar q, t) + e(p - \hbar q, t)].
\]

We now assume that the atoms are initially in the ground state with momentum \( p_0 = 0 \), so that the initial wave function is

\[
|\psi(p, 0)\rangle = g(0, 0)|g\rangle.
\]

In the case \( \delta \ll \mathcal{R} \) the detuning term \( -\hbar \delta e(p, t) \) in equation (2.6) can be neglected [38], leading to the set of equations

\[
i\hbar \dot{e}(p, t) = \frac{\hbar \mathcal{R}}{2} [g(p + \hbar q, t) + g(p - \hbar q, t)],
\]
CHAPTER 2. COHERENT INTERACTION

\begin{equation}
\frac{i\hbar}{2} \gamma(p, t) = \frac{\hbar \mathcal{R}}{2} [e(p + \hbar q, t) + e(p - \hbar q, t)], \tag{2.9}
\end{equation}

for which it proves convenient, to express \( g(p, t) \) and \( e(p, t) \) as the discrete series

\begin{align*}
e(p, t) &= \sum e_m(t) \delta(p - p_0 - m\hbar q), \tag{2.10} \\
g(p, t) &= \sum g_m(t) \delta(p - p_0 - m\hbar q). \tag{2.11}
\end{align*}

Noting that for the initial condition (2.8) the sum (2.11) effectively ranges over even values of \( m \), while the sum (2.10) ranges over odd values of \( m \), we introduce the new variable \( x_m(t) \) such that

\begin{equation}
x_m(t) = \begin{cases} 
e_m(t), & (m \text{ odd}), \\
g_m(t), & (m \text{ even}), 
\end{cases} \tag{2.12}
\end{equation}

to finally obtain

\begin{equation}
\frac{i\hbar}{2} \dot{x}_m = \frac{\hbar \mathcal{R}}{2} (x_{m-1} + x_{m+1}) \tag{2.13}
\end{equation}

for the amplitudes \( x_m \). The solutions to this equation are given in terms of the well known \( n^{th} \)-order Bessel functions of the first kind \( J_n() \) [38].

In the case \( \delta \gg \mathcal{R} \) the probability amplitude for the upper electronic level of the atom can be adiabatically eliminated from the Schrödinger equation (2.6)–(2.7) by a standard procedure [32], leading to the scalar equation

\begin{equation}
\frac{i\hbar}{\delta} \gamma(p, t) = \frac{\gamma R^2}{\delta} g(p, t) + \frac{\hbar \mathcal{R}^2}{2\delta} [g(p + 2\hbar q, t) + g(p - 2\hbar q, t)]. \tag{2.14}
\end{equation}
CHAPTER 2. COHERENT INTERACTION

With the phase transformation

$$\tilde{g}(p, t) = g(p, t)e^{i\mathcal{R}^2 t/\delta}$$  \hspace{1cm} (2.15)

and the expansion

$$\tilde{g}(p, t) = \sum_m x_m(t)\delta(p - p_0 - 2m\hbar q)$$  \hspace{1cm} (2.16)

we can write equation (2.14) as

$$i\hbar \dot{x}_m = \frac{\hbar \mathcal{R}^2}{2\delta}[x_{m-1} + x_{m+1}],$$  \hspace{1cm} (2.17)

similar to Eq. (2.13). The solutions are again given in terms of the $n$th-order Bessel functions of the first kind $J_n()$. Note however the factor 2 in the expansion (2.16) compared to the factor 1 in expansions (2.11) and (2.10). It is a result of the virtual (2-photon) transitions induced by a large detuning.

Particularly, the probability $P_m$ to find the atom deflected with momentum $m\hbar q$ after an interaction time $\tau$ is given by

$$P_m = J_m^2(\mathcal{R}\tau)$$  \hspace{1cm} (2.18)

for $\delta \ll \mathcal{R}$, and by

$$P_{2m} = J_m^2\left(\frac{\mathcal{R}^2}{2\delta}\tau\right)$$  \hspace{1cm} (2.19)

for $\delta \gg \mathcal{R}$. To be consistent with the Raman-Nath approximation, the kinetic energy ac-
CHAPTER 2. COHERENT INTERACTION

quired by the atom during the interaction must remain small, which imposes the conditions [38, 32]

\[ \tau \ll \frac{1}{\sqrt{R \omega_{rec}}} \quad (2.20) \]

for \( \delta \ll R \), and

\[ \tau \ll \frac{\sqrt{2 \delta \omega_{rec}}}{R} \quad (2.21) \]

for \( \delta \gg R \).

In the Raman-Nath regime we can also make predictions about the spread of the momentum with time. The root mean square momentum

\[ \sqrt{\langle p^2 \rangle} = \left[ \hbar^2 q^2 \sum_m m^2 p_m^2 \right] \quad (2.22) \]

is approximately given by [37]

\[ \sqrt{\langle p^2 \rangle} \approx R \tau \quad (2.23) \]

for \( \delta \ll R \), and

\[ \sqrt{\langle p^2 \rangle} \approx \frac{R^2}{\delta} \tau \quad (2.24) \]

for \( \delta \gg R \).

We later illustrate this linear dependence of the root-mean-square momentum on the interaction time with computer simulations, which also show that the linear dependence breaks down drastically when the interaction time ceases to fulfill conditions (2.20) and
2.1.2 Two-Beam Resonances

For certain parameter regions, the kinetic energy term of the Hamiltonian (2.1) serves as a phase matching mechanism. This effectively restricts the diffraction orders that the atomic wave function can scatter into, in sharp contrast to the linear increase of the root-mean-square momentum in the Raman-Nath regime that we discussed above.

Of particular interest are the two-beam resonances, for which two atomic momentum states are strongly coupled, leading during the interaction to a periodic exchange of their probabilities. A requirement for these resonances to occur is that the energies of the two momentum states involved are about the same. This suggests as one possible pair of states two atomic states with opposite momenta and same electronic excitation.

As an example, the experimental parameters could be set to values which ensure that an incoming atom with momentum $p = 2\hbar q$ leaves the interaction region with $p = -2\hbar q$. Alternatively, the interaction time could be adjusted so that the atom leaves the interaction region with an equal probability to have the momenta $p = 2\hbar q$ and $p = -2\hbar q$. In the latter case the laser field acts effectively as a atomic beam-splitter. We will investigate these two-beam resonances in detail in section 2.2.4.

Before proceeding with examples, we discuss a universal approach to the atomic scattering problem described by the Hamiltonian (2.1) that we developed to (i) provide a deeper understanding of the system, (ii) facilitate the numerical implementation of the problem,
and (iii) allow the inclusion of spontaneous emission.

2.2 Band Theoretical Approach

The periodic interaction (2.1) suggests applying the band-theoretical approach of solid state physics to solve the time-independent Schrödinger equation

\[ E|\psi\rangle = H|\psi\rangle \]  

(2.25)

for the Hamiltonian (2.1) with the rectangular beam profile (2.2), effectively treating the standing-wave laser field as a light crystal [40]. As we shall see, this approach provides us with a formalism that can readily be used for a numerical implementation of the problem. Furthermore, it provides useful insight into the properties and resonances of the model.

2.2.1 Symmetries

We first observe that the Hamiltonian (2.1) is invariant under the unitary transformation \( T \),

\[ T : \left( \sigma_1 \rightarrow -\sigma_1, x \rightarrow x + \frac{\pi}{q} \right), \]  

(2.26)

which involves the inversion of the atomic polarization concomitant with a displacement of the atom by a half wavelength of the electromagnetic field. By virtue of the formal identities

\[ e^{\frac{\pi}{q} \frac{d}{dx}} f(x) = f(x + \frac{\pi}{q}), \]  

(2.27)
and

\[ \sigma_3 \sigma_1 \sigma_3 = -\sigma_1, \quad (2.28) \]

the transformation \( T \) may be represented by the unitary operator

\[ T = \sigma_3 e^{i \frac{\pi}{\hbar} \hat{\rho}} \quad (2.29) \]

in terms of which the invariance of \( H \) under the unitary transformation \( T \) reads

\[ [H, T] = 0. \quad (2.30) \]

This expresses the fact that \( H \) and \( T \) possess a common system of eigenstates.

The diagonalization of \( T \) is performed easily by noting that the set of electro-translational states

\[ |\kappa, m\rangle = \begin{cases} |\kappa + mq\rangle \otimes |g\rangle & \text{if } m \text{ even}, \\ |\kappa + mq\rangle \otimes |e\rangle & \text{if } m \text{ odd}, \end{cases} \quad (2.31) \]

are eigenstates of \( T \),

\[ T|\kappa, m\rangle = - e^{i \frac{\pi \kappa}{\hbar}} |\kappa, m\rangle. \quad (2.32) \]

The quasi-wavenumber \( \kappa \) is the Floquet exponent of \( T \). In equation (2.31),

\[ \langle x| \kappa + mq \rangle = \frac{1}{\sqrt{2\pi}} e^{i (\kappa + mq)x} \quad (2.33) \]
is a plane wave with wave number \( k = \kappa + mq \). To provide for a unique parametrization of the eigenvalue \(-e^{i(\pi/q)\kappa}\) of \( T \) the quasi-wave-number \( \kappa \) needs to be restricted to a Brillouin zone of size \( 2q \). We choose the first Brillouin zone, defined by \(-q \leq \kappa < q\). With this restriction, the set of atomic electro-translational states \( \{ |\kappa, m\rangle, m = 0, \pm 1 \pm 2 \ldots \} \) is orthonormal,

\[
\langle \kappa', m' | \kappa, m \rangle = \delta_{m,m'} \delta(\kappa - \kappa'),
\]

and complete

\[
\sum_n \int_{-q}^{q} dk |\kappa, m\rangle \langle \kappa, m| = 1.
\]

It is important to note, that there also exists a subgroup of the symmetry group generated by \( T \), which is generated by \( T^2 = e^{i(2\pi/q)(d/dx)} \). This subgroup represents the more obvious \( x \rightarrow x + 2\pi/q \) invariance of the interaction [41, 42]. However, the corresponding Brillouin zone would be twice as large as the one prescribed by the full symmetry group \( T \).

2.2.2 Expansion of the Eigenstates of \( H \)

Besides being eigenstates of \( T \), the electro-translational states (2.31) are eigenstates of the free Hamiltonian as well,

\[
\left( \frac{p^2}{2M} - \hbar \delta |e\rangle \langle e| \right) |\kappa, m\rangle = E^{(0)}_m(\kappa) |\kappa, m\rangle.
\]
The eigenvalues
\[ E_m^{(0)}(\kappa) = \frac{\hbar^2 (\kappa + m q)^2}{2M} - \frac{1 - (-1)^m}{2} \hbar \delta \] (2.37)
give the dispersion branches of the free atom as a function of \( \kappa \) and \( m \). For \( m \) even (odd) the branches refer to the atom with momentum \( p = \hbar (\kappa + m q) \) in the electronic state \( |g\rangle \) \((|e\rangle\)). Figure 2.2 displays the first few branches of the free atom’s dispersion relation

![Dispersion Relation Diagram](image)

**Figure 2.2:** Branches of the dispersion relation of the free atom as a function of the quasi-wavenumber \( \kappa \) (in units of \( E_{\text{rec}} \) and \( q \), respectively). The thickened lines in bands 2 and 0 indicate the possible final states for a free two-level atom with an initial state indicated by the dot in band 1, decaying into the ground state via spontaneous emission (see section 3.1).

(2.37) in the first Brillouin zone. The branches with indices \( m = 0, \pm 2, \pm 4, \ldots \) refer to the
atom in the state $|g\rangle$, while the branches with indices $m = \pm 1, \pm 3, \ldots$ refer to the atom in the state $|e\rangle$. The dispersion relation of the atom in state $|e\rangle$ is displaced vertically by the detuning energy $\hbar\delta$, and horizontally by $q$, the wave number of the electromagnetic field. The intersections of two branches lead to two-beam resonances, as we will discuss in section 2.2.4. Note that for the coherent interaction considered in this chapter only vertical transitions between bands are allowed, since the atomic quasi-momentum $\kappa$ is conserved.

Every eigenstate $|\phi_\nu(\kappa)\rangle$ of the Hamiltonian (2.1) may be expanded in a Fourier series

$$|\phi_\nu(\kappa)\rangle = \sum_{m=-\infty}^{\infty} \chi_{m\nu}(\kappa) |\kappa, m\rangle \tag{2.38}$$

with expansion coefficients

$$\langle \kappa', m | \phi_\nu(\kappa) \rangle = \delta(\kappa - \kappa') \chi_{m\nu}(\kappa). \tag{2.39}$$

The Kronecker Delta function $\delta(\kappa - \kappa')$ in this equation is due to the fact that $\kappa$ is a good quantum number.

In terms of the expansion coefficients $\chi_{m\nu}(\kappa)$ the stationary Schrödinger equation (2.25) becomes

$$E_\nu(\kappa)\chi_{m\nu}(\kappa) = E^{(0)}_m(\kappa)\chi_{m\nu}(\kappa) + \hbar \frac{\mathcal{R}}{2} (\chi_{m+1,\nu}(\kappa) + \chi_{m-1,\nu}(\kappa)), \ m = 0, \pm 1, \pm 2, \ldots \tag{2.40}$$

This is a scalar tridiagonal recurrence relation very similar to the Fourier representation
of the Mathieu equation [43]. For a given \( \kappa \), the set of equations (2.40) has infinitely many solutions \( E_\nu(\kappa), \chi_{\nu,m}(\kappa), m = 0, \pm 1, \pm 2, \ldots \), which are enumerated by a band index \( \nu = 0, 1, 2, \ldots \) so that \( E_{\nu'}(\kappa) > E_{\nu}(\kappa) \) for \( \nu' > \nu \). Solutions can easily be obtained by means of a continued-fraction method [44], or by a suitably truncated matrix diagonalization.

Figure 2.3: Band scheme of the Hamiltonian (2.1) for \( R = 2 \) and \( \delta = 1/2 \) (in units of \( \omega_{\text{rec}} \)). The apparent crossings in the upper part of the band scheme are actually avoided crossings.

Figure 2.3 displays the first few energy bands \( E_\nu(\kappa) \) for the Hamiltonian (2.1) for \( R = 3\omega_{\text{rec}} \) and \( \delta = 1/2\omega_{\text{rec}} \). Comparing this figure with Fig. 2.2, two major changes can be observed: One is a small vertical shift of the electro-translational levels (AC Stark shift), the other is the appearance of band gaps (level repulsion) wherever two branches of the
dispersion relation of the free atom intersect.

2.2.3 Time Evolution

Once the coefficients $\chi_{nm}(\kappa)$ have been calculated, the time evolution is given by

$$|\psi(t + \Delta t)\rangle = U|\psi(t)\rangle$$  \hspace{1cm} (2.41)

with the unitary time evolution operator $U \equiv e^{-\frac{i}{\hbar}H\Delta t}$. We can use the eigenfunctions $|\phi_{\nu}(\kappa)\rangle$ of $H$ to write

$$U = \int_{-q}^{q} d\kappa \sum_{\nu} e^{-\frac{i}{\hbar}E_{\nu}(\kappa)\Delta t}|\phi_{\nu}(\kappa)\rangle\langle\phi_{\nu}(\kappa)|.$$  \hspace{1cm} (2.42)

The matrix elements of $U$ are given by

$$\langle\kappa, m|U|\kappa', m'\rangle = \delta(\kappa - \kappa')U_{m,m'}(\kappa)$$  \hspace{1cm} (2.43)

with (see Eq. (2.38))

$$U_{m,m'}(\kappa) = \sum_{\nu} e^{-\frac{i}{\hbar}E_{\nu}(\kappa)\Delta t}\chi_{m\nu}(\kappa)\chi_{m'\nu}^{*}(\kappa).$$  \hspace{1cm} (2.44)
CHAPTER 2. COHERENT INTERACTION

The completeness of the electro-translational states $|\kappa, m\rangle$ guarantees, that we can expand the wave function $|\psi(t)\rangle$ in plane wave components,

$$|\psi(t)\rangle = \int_{-q}^{q} d\kappa \sum_{m} C_{m}(\kappa, t)|\kappa, m\rangle,$$

(2.45)

where

$$P(p = \hbar(\kappa_{0} + mq)) \equiv |C_{m}(\kappa_{0}, \tau)|^{2}$$

(2.46)

denotes the probability for the atom to have the momentum $p = \hbar(\kappa_{0} + mq)$. Combining Eqs. (2.41)-(2.45) we can finally write the time evolved state vector as

$$|\psi(t + \Delta t)\rangle = \int_{-q}^{q} d\kappa \sum_{m} C_{m}(\kappa, t + \Delta t)|\kappa, m\rangle,$$

(2.47)

where

$$C_{m}(\kappa, t + \Delta t) = \sum_{m'} U_{m,m'}(\kappa)C_{m'}(\kappa, t).$$

(2.48)

For our rectangular beam profile (2.2) the coefficients $C_{m'}(\kappa, t)$ describe the population of the eigenstates of the free hamiltonian $H_{0}$ before the atom enters the interaction region, while the coefficients $C_{m}(\kappa, t + \tau)$ describe the final momentum distribution after an interaction time $\tau$, according to equation (2.46).

To treat a more general Gaussian beam envelope with the same method, we would simply divide the interaction time into multiple time-steps, each small enough to resolve the beam envelope and to justify the approximation $H \approx \text{const.}$ for the time between the
steps. Note, that the coefficients $\chi_{m\nu}(\kappa)$ have to be reevaluated for each time step since the Hamiltonian (2.1) changes its value.

So far we have described the general dynamics of the atomic momentum distribution, and we turn now to the discussion of the resonances.

2.2.4 Two-Beam Resonances

As we have seen in section 2.2.2, the atom-field interaction leads to level repulsion in the band scheme of the free two-level atom (see Fig 2.2) wherever two branches cross, combined with a AC Stark shift. Figure 2.4 gives a detailed illustration of the level repulsion between two bands, $E_{\nu'}$, $E_{\nu'+1}$ near an intersection of two branches $E_{m_0}^{(0)}$, $E_{m_1}^{(0)}$ of the free-atom.

Figure 2.4: Level repulsion near an intersection of two branches of the free atom.
dispersion relation. The two branches cross at values \( \kappa_r^{(0)} \) and \( E_r^{(0)} \) defined by

\[
E_r^{(0)} \equiv E_{m_0}^{(0)}(\kappa_r^{(0)}) = E_{m_1}^{(0)}(\kappa_r^{(0)}).
\]  

From neutron diffraction \[45\] we know that we can get two-beam resonances whenever (i) the energy of the deflected atom approximately equals the energy of the undeflected atom, and (ii) the energy differences between all scattering orders except these two are large compared to the atom-laser interaction energy. Condition (i) ensures that the transition between the undeflected and the deflected state is energetically allowed, and is realized at all level crossings in the band scheme of the free two-level atom (see Fig 2.2). Condition (ii) ensures that all other diffraction orders remain unpopulated due to their energy mismatch. It can be realized in our case with a coupling constant \( \mathcal{R} \) that is not too strong.

If these conditions are fulfilled, the eigenstates far away from a resonance are approximately given by the electro-translational states of the noninteracting Hamiltonian \( H_0 \). In the vicinity of the resonances, however, the two electro-translational states with near-degenerate energies representing the deflected and the undeflected beams become strongly coupled. The eigenstates \( |\phi_{\nu'}\rangle \), \( |\phi_{\nu'+1}\rangle \) and the corresponding eigenvalues \( E_{\nu'}, E_{\nu'+1} \) at the resonance may be calculated by means of a continued fraction method where all but the two potentially degenerate levels \( |\kappa, m_0\rangle \), \( |\kappa, m_1\rangle \) in Eq. (2.40) are eliminated \[40\]. In the resulting two-level approximation we can write in the presence of interaction (dressed
states) for $\kappa_r = \kappa_r^{(0)} + \epsilon_r$ (near crossings)

$$
|\phi_{\nu'+1}\rangle = \frac{1}{\sqrt{2}}(\kappa_r, m_0) + s|\kappa_r, m_1\rangle, \\
|\phi_{\nu}\rangle = \frac{1}{\sqrt{2}}(\kappa_r, m_0) - s|\kappa_r, m_1\rangle
$$

(2.50)

where $s = \pm 1$ determines the parity of the eigenstates and their eigenvalues, and $\epsilon_r$ is a possible small shift in $\kappa$ due to the AC-Stark shift.

We are mainly interested in the dynamical behavior of the resulting dressed state system (2.50). If the transverse momentum of the incoming atom is, e.g., in the state $|\kappa_r, m_0\rangle$ of Eq. (2.50) then upon entering the field the bare atomic wave function may be expressed as the coherent superposition

$$
|\phi(0)\rangle = |\kappa_r, m_0\rangle \\
= \frac{1}{\sqrt{2}}(|\phi_{\nu}\rangle + |\phi_{\nu'+1}\rangle)
$$

(2.51)

of the dressed states (2.50). While the atom is inside the laser beam, the state vector evolves according to

$$
|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left( e^{-\frac{i}{\hbar}E_{\nu}t}|\phi_{\nu}\rangle + e^{-\frac{i}{\hbar}E_{\nu'+1}t}|\phi_{\nu'+1}\rangle \right),
$$

(2.52)

so that the probability to find the atom scattered into the state $|\kappa_r, m_1\rangle$ when the atom
leaves the laser beam after an interaction time \( \tau \), is given by

\[
P_1 = \frac{1}{2} \left[ 1 - \cos\left( \frac{\Delta E \tau}{\hbar} \right) \right]. \tag{2.53}
\]

Here

\[
\Delta E = E_{\nu'+1}(\kappa_r) - E_{\nu}(\kappa_r) \tag{2.54}
\]
denotes the energy difference between the two dressed states (band gap). The probability to find the atom undeflected is \( P_0 = 1 - P_1 \). As a function of the interaction time \( \tau \), the diffraction probabilities \( P_0 \) and \( P_1 \) show the typical oscillations of the Pendellösung [39, 30, 46, 47]. In particular, for the interaction time

\[
\tau_{\text{split}} = \frac{\pi}{2\Delta E} \tag{2.55}
\]

the standing-wave operates as a 50/50 atomic beam splitter. To gain a deeper understanding of the two-beam resonances, and to predict the frequency of the oscillations, we need to precisely derive the resonance conditions, and calculate the energy difference \( \Delta E = E_{\nu'+1}(\kappa_r) - E_{\nu}(\kappa_r) \) in terms of the various experimental parameters.

**Bragg and Doppleron Resonances**

Two kinds of resonances have been discussed and observed in the past: Bragg resonances and Doppleron resonances. A glance at figure 2.2 reveals that the band scheme is characterized
by two families of bands which represent the two electronic states $|e\rangle$ and $|g\rangle$. These two families give rise to inter-family and intra-family level crossings, which behave differently as the detuning $\delta$ is varied, and which lead to so-called Bragg and Doppleron resonances [39, 30, 46, 48, 49].

Bragg resonances are associated with intra-family crossings, i.e. diffraction processes that leave the electronic state of the atom unchanged (see Fig. 2.3). They appear exclusively at the center ($\kappa = 0$) and the boundaries ($\kappa = \pm q$) of the Brillouin zone, and they do not change their position in the Brillouin zone when the atom-field detuning $\delta$ is changed. Bragg resonances are, like their counterparts in solid state physics and optics, of purely geometrical origin.

Doppleron resonances on the other hand are associated with inter-family crossings i.e. diffraction processes that change the electronic state of the atom (see Fig. 2.3). These crossings can be located anywhere throughout the entire Brillouin zone, and they change their position with varying detuning $\delta$. Doppleron resonances are also called velocity-tuned resonances, since for a given detuning the atomic velocity (i.e. $m_0, \kappa_r$) has to be properly selected to achieve level crossing.

Bragg resonances of order $l$ couple momentum eigenstates with $p = \pm hlq$, and involve $2l$ photon transitions. As shown in Appendix C, the conditions for a Bragg resonance to occur are, aside from the geometrical requirement $\kappa = 0, \pm q$ (condition (i)), usually called
the "Bragg-condition") either a sufficiently weak interaction,

$$\delta \ll R \ll \omega_{rec},$$  \hspace{1cm} (2.56)

or a sufficiently strong detuning

$$\delta \gg R, \frac{R^2}{4\omega_{rec}}$$  \hspace{1cm} (2.57)

(condition (ii)). The better condition (2.56) or (2.57) is fulfilled, the weaker the diffraction orders due to levels other than \(|\kappa_r, m_o\rangle\) and \(|\kappa_r, m_1\rangle\), and the cleaner the resonance.

The regime of large detunings, \(\delta \gg R, \frac{R^2}{4\omega_{rec}}\), is of particular practical importance, since it corresponds to situations where the upper electronic state remains weakly populated if the incoming atom is in the lower electronic state. The atom behaves in this case like a scalar particle interacting with the periodic potential provided by the standing laser wave. This scalar nature holds of course also for atoms initially in their excited state since we here consider only the coherent, reversible evolution.

The energy gap \(\Delta E_{Bragg}\) of Eq. (2.54) for Bragg resonances may be calculated following standard methods. Appendix C shows the calculation for \(\delta \gg R, \frac{R^2}{4\omega_{rec}}\) which results in

$$\Delta E_{Bragg} \approx 2\hbar\omega_{rec}\frac{(\frac{R^2}{\Delta\omega_{rec}})^l}{4(l-1)((l-1)!)^2},$$  \hspace{1cm} (2.58)

Doppleron resonances couple momentum states with \(p_0 = \hbar(\kappa_r + m_0q)\) and \(p_1 = \hbar(\kappa_r + (m_0 + 2l + 1)q)\) via a \(2l + 1\) photon transition, where \(l\) labels the order of the resonance. For
simplicity we discuss only the $l^{th}$-order Doppleron resonance with $\kappa_r = 0$, in which an atom in the ground (upper) state with transverse momentum $p_0 = \hbar m_0 \mathbf{q}$ is resonantly scattered into a state where the atom is in the upper (ground) state, and moves with transverse momentum $p_1 = \hbar (m_0 + 2l + 1) \mathbf{q}$ ($p_1 = \hbar (m_0 - 2l - 1) \mathbf{q}$). We also assume $m_0 \gg l > 0$, so that the Bragg scattering between $p_0$ and $-p_0$ which is also present for $\kappa_r = 0$ does not play a role on the time scale of the Doppleron scattering between $p_0$ and $p_1$.

The role of the Bragg "geometric" condition $\kappa = 0, \pm 1$ (condition (i), Eq. (2.49)) is for Doppleron resonances replaced by a condition for the detuning $\delta_r$ depending on the initial transverse momentum $p_0 = \hbar m_0 \mathbf{q}$, the Rabi frequency $\mathcal{R}$, and the order $l$ of the resonance. To zeroth order in the atom-laser coupling this condition may be written as

$$\delta_r^{(0)}/\omega_{rec} = (m_0 + 2l + 1)^2(-1)^{m_0} - m_0^2(-1)^{m_0}. \quad (2.59)$$

Taking into account the atom-laser interaction, this resonance condition is modified due to AC-Stark shifts induced by the non-resonant electro-translational levels, as a detailed calculation discussed in Appendix C shows. The general expression for the detuning $\delta_r$ is quite complicated, and does not provide much physical insight. As an example, we reproduce here its particular value for a second-order Doppleron ($l = 2$) [50],

$$\delta_r/\omega_{rec} = (m_0 + 5)^2 - m_0^2 + \frac{5\mathcal{R}^2}{96\omega_{rec}^2} \left[ \frac{N_1 + N_2}{m_0 + 2} + \frac{N_3 + N_4}{m_0 + 3} \right]. \quad (2.60)$$

The constants $N_1$--$N_4$ are numbers of order one whose full expressions in terms of $m_0$ and
\( \mathcal{R} \) are also given in Appendix C.

The calculation in Appendix C further shows that in order to suppress a multiple beam situation (condition (ii)), the Rabi frequency must satisfy the inequality

\[
\mathcal{R} \ll 8m_0\omega_{\text{rec}}. \tag{2.61}
\]

This is the Doppleron equivalent of conditions (2.56, 2.57) for the Bragg resonances. The energy gap for Doppleron resonances is given by

\[
\Delta E_{\text{Doppler}} = \hbar \mathcal{R} \left( \frac{\mathcal{R}}{8\omega_{\text{rec}}} \right)^l m_0! \frac{1}{\left( \frac{3}{2} + l \right)!}. \tag{2.62}
\]

Compared with the corresponding expression (2.58) for a \( l^{\text{th}} \) order Bragg resonances, equation (2.62) reveals the potential advantage of a Doppleron resonance. In terms of the smallness parameter \( \epsilon \) of the resonances (see conditions (2.56)–(2.57) and (2.61)), the energy gap for the Bragg resonance scales as \( \Delta E_{\text{Bragg}} \sim \hbar \omega_{\text{rec}} \epsilon^l \) with \( \epsilon = \mathcal{R}^2/4\delta \omega_{\text{rec}} \), while for the Doppleron resonance it scales as \( \Delta E_{\text{Doppler}} \sim \hbar \mathcal{R} \epsilon^l \) with \( \epsilon = \mathcal{R}/8m_0\omega_{\text{rec}} \). For fixed \( \epsilon < 1 \), the energy gap of a Doppleron resonance increases with increasing \( \mathcal{R} \), indicating that the splitting time \( \tau_{\text{split}} \) (Eq. (2.55)) may become significantly faster for Doppleron resonances than for the Bragg resonances.
Examples

Figure 2.5 displays the time-evolution of a first-order Bragg-resonance in the absence of spontaneous emission. The incoming atom is in its ground state, and the initial transverse momentum is \( p_0 = \hbar q \). The interaction parameters are close to those used in the experiments of Martin et al. [30], namely \( \mathcal{R} = 385\omega_{\text{rec}} \) and \( \delta = 32000\omega_{\text{rec}} \). Although the full set of equations (2.40) was solved to obtain the results displayed in that figure, the inequality \( \delta \gg \mathcal{R} \) would have allowed to use the much simpler description of Bragg resonances derived in Appendix C. However, the smallness parameter \( \epsilon = \mathcal{R}^2/4\delta\omega_{\text{rec}} = 1.15 \) is already larger than one, which explains the appearance of (undesired) diffraction side orders with momenta \( \pm 3\hbar q \). The energy gap \( \Delta E = 2\epsilon E_{\text{rec}} \) implies a split-time \( \tau_{\text{split}} = h\pi/2\Delta E = 0.68/\omega_{\text{rec}} \), which agrees well with the corresponding time that can be read off figure 2.5. The result of a simulation with the same parameters, but with the atom initially in the lower electronic state is indistinguishable from the result displayed in Fig 2.5, since the interaction described by the Hamiltonian (2.1) is symmetric with respect to an interchange of the electronic levels and a sign change of the detuning.

Figure 2.6 displays the time evolution of a second-order Doppleron resonance. The incoming atom is in its ground state with momentum \( p_0 = 660\hbar q \) [51]. The Rabi-frequency is \( \mathcal{R} = 4000\omega_{\text{rec}} \), and the value of the detuning has been chosen according to equation (2.62) to obtain an optimal two beam resonance, namely \( \delta = 3640.35\omega_{\text{rec}} \).

The value of the parameter \( \epsilon = \mathcal{R}/(8m_0\omega_{\text{rec}}) \), which indicates how well the two beam resonance is realized, is \( \epsilon = 0.76 \) for this situation. This is not very small compared to 1,
Figure 2.5: Pendellösung effect without spontaneous emission. The atom is initially in the lower state and $p_0 = 1$, $\mathcal{R} = 385$, $\delta = 32000$ and $\Gamma = 0$ (in units of the recoil frequency $\omega_{\text{rec}}$). The parameters are the same as for the experimental data shown in figure 2(a) of Martin et al. [30].

which explains the various fast oscillations visible in the graph, as well as the somewhat modest population transfer of at most $\approx 65\%$ to $p_1 = 665\hbar q$. Note however, that the transfer time $2\tau_{\text{split}} \approx 0.009/\omega_{\text{rec}}$ is appealingly small. To achieve a similar momentum transfer with a Bragg resonance (either 4 or 6 $\hbar q$), times of the order of $\tau \approx 10 - 100/\omega_{\text{rec}}$ would be necessary (using the same $\mathcal{R}$). This underlines the advantage of Dopplerons for beam splitter applications. Before drawing definitive conclusions however, we need to consider the potentially devastating impact of spontaneous emission. We will do this in section 3.2.

To demonstrate the vast improvement of the Doppleron resonances with decreasing
Figure 2.6: Second order Doppleron resonance with the parameters $p_0 = 660, g = 4000, \delta = 3640.35$ without spontaneous emission ($\Gamma = 0$, frequencies in units of $\omega_{rec}$). The atom is initially in its lower state. The momentum transfer is not very effective, and has a peak of about 63%. Note however the small transfer time of $\tau \approx 0.09$.

$\epsilon = \mathcal{R}/(8m_0\omega_{rec})$, a rather clean Doppleron resonance with $p_0 = 1320\hbar q$ and $p_1 = 1325\hbar q$ is displayed in figure 2.7. Here $\epsilon$ has been reduced by a factor of 2 as compared to the previous example. To keep the resonance fast, we increased $m_0$ rather than decreasing $\mathcal{R}$ since $\epsilon \sim \mathcal{R}/m_0\omega_{rec}$, while $\tau_{split} \sim m_0^4\omega_{rec}^4/\mathcal{R}^3$. The detuning is chosen from Eq. (2.62) as $\delta = 11925.4\omega_{rec}, \mathcal{R} = 4000\omega_{rec}$, and $\Gamma = 0$. Compared with figure 2.6, figure 2.7 shows a resonance which is much less perturbed by side diffraction orders. However, the split time $\tau_{split}$ is now a factor $2^4$ larger than in figure 2.6.
Figure 2.7: Improved second order Doppleron resonance with the parameters $p_0 = 1320, g = 4000, \delta = 11925.4$ without spontaneous emission ($\Gamma = 0$, frequencies in units of $\omega_{rec}$). The atom is initially in its lower electronic state. The momentum transfer is now much more effective than in figure 2.6 ($\approx 92\%$ at peak), but at the cost of a longer transfer time.

### 2.3 Quantum Fields

Recent advances in cavity QED [52] have raised the prospects to perform atomic beam deflection experiments with fields of low photon numbers, which require a quantum description. In this section we investigate some effects of the granular nature of fields on atomic diffraction.

Assuming that the field used to diffract the atoms is a single mode, standing wave, the
total Hamiltonian of the atom-field system is given by

\[ \mathcal{H}_Q = \frac{p^2}{2M} + \hbar \omega |e\rangle \langle e| + \hbar \Omega a^\dagger a + \hbar g f(t) \cos \varphi \hat{\sigma}_+(a + a^\dagger). \]  \hspace{1cm} (2.63)

Here \( g = \sqrt{\frac{\mu}{\varepsilon_0 \omega V}} \), where \( \sqrt{\frac{\mu}{\varepsilon_0 \omega V}} \) is the electric field per photon in a mode volume \( V \), and \( \Omega \) is the frequency of the field. We use again the rectangular mode profile (2.2). The annihilation and creation operators \( a \) and \( a^\dagger \) obey the usual commutation relation \([a, a^\dagger] = 1\).

In an interaction picture defined by the unitary transformation

\[ U = e^{-i\mathcal{H}t(a^\dagger e + |e\rangle \langle e|)}, \]  \hspace{1cm} (2.64)

and in the rotating wave approximation, the interaction Hamiltonian becomes

\[ H_Q = \frac{p^2}{2M} - \hbar \delta |e\rangle \langle e| + \hbar g f(t) \cos \varphi \hat{\sigma}_+(a + a^\dagger), \]  \hspace{1cm} (2.65)

where \( \delta = \Omega - \omega \) is the detuning between the mode frequency \( \Omega \) and the atomic transition frequency \( \omega \).

### 2.3.1 Extension of the Band Theory to Quantum Fields

The band-theoretical description developed in section 2.2 for classical fields can readily be extended to quantum fields. To do this, we consider again the stationary Schrödinger
equation

\[ H_Q |\psi\rangle = E |\psi\rangle. \]  (2.66)

Just as the semiclassical Hamiltonian (2.1), the Hamiltonian (2.65) is invariant under the unitary transformation \( T \) defined in (2.26), i.e.

\[ [H_Q, T] = 0. \]  (2.67)

Furthermore the operator

\[ W \equiv \sigma_+ \sigma_- + a^\dagger a \]  (2.68)

which measures the combined excitation of the field and the electronic state of the atom, commutes with both \( H_Q \) and \( T \),

\[ [H_Q, W] = 0, [W, T] = 0, \]  (2.69)

i.e. \( W \) is also a constant of motion. Mathematically, Eqs. (2.67)–(2.69) imply that \( H_Q, T \) and \( W \) have a common set of eigenstates. Using arguments similar to those of section 2.2.1, the diagonalization of \( T \) and \( W \) is performed by noting that the states

\[ |\kappa, m, N\rangle = \begin{cases} |\kappa + mq\rangle \otimes |g\rangle \otimes |n = N\rangle, & \text{m even, } N = 0, 1, \ldots, \\ |\kappa + mq\rangle \otimes |e\rangle \otimes |n = N - 1\rangle, & \text{m odd, } N = 1, 2, \ldots, \end{cases} \]  (2.70)
are eigenstates of $T$,

$$T|\kappa, m, N\rangle = e^{-i\frac{\pi}{2} \kappa}|\kappa, m, N\rangle, \quad (2.71)$$

and $W$,

$$W|\kappa, m, N\rangle = N|\kappa, m, N\rangle. \quad (2.72)$$

In Eq. (2.70) $|n\rangle$ indicates a fock state with $n$ photons, and

$$\langle x|\kappa + mq\rangle = \frac{1}{\sqrt{2\pi}} e^{i(\kappa + mq)x}, \quad (2.73)$$

is a plane wave with wave number $\kappa + mq$.

From Eqs. (2.71) and (2.72) we infer that both the atomic quasi-wave-number $\kappa$ and the excitation number $N$ are good quantum numbers. As before, we limit the values of $\kappa$ to the first Brillouin zone, $-q \leq \kappa < q$. With this limitation, the set of electro-translational-field states $\{|\kappa, m, N\rangle| m = 0, \pm 1, \pm 2, \ldots, N = 0, 1, 2, \ldots \}$ is orthonormal,

$$\langle \kappa', m', N'|\kappa, m, N\rangle = \delta(\kappa - \kappa') \delta_{m,m'} \delta_{N,N'}, \quad (2.74)$$

and complete

$$\sum_{m,N} \int_{-q}^{q} d\kappa |\kappa, m, N\rangle \langle \kappa, m, N| = 1. \quad (2.75)$$

From equations (2.67) and (2.69), the states (2.70) are also eigenstates of the free part of
the Hamiltonian (2.65),

$$\left( \frac{p^2}{2M} - \hbar \delta |e\rangle \langle e| \right) |\kappa, m, N\rangle = E^{(0)}_m(\kappa) |\kappa, m, N\rangle.$$  \tag{2.76}

Here

$$E^{(0)}_m(\kappa) = \frac{\hbar^2 (\kappa + mq)^2}{2M} - \frac{1 - (-1)^m}{2} \hbar \delta, \ m = 0, \pm 1, \pm 2 \ldots \tag{2.77}$$

give the dispersion branches of the free atom. Since we have effectively transformed away the free field energy with the transformation (2.64), the dispersion relation (2.77) is the same as that discussed in section 2.2.2. and displayed in Fig. (2.2).

The observation that $N$ is a good quantum number expresses the fact, that the interaction part $H_I = \hbar g \cos q x (\sigma_+ a + \sigma_- a^\dagger)$ of the Hamiltonian $H_Q$ conserves not only the atomic quasi-momentum $\kappa$, but also the total excitation number $N$,

$$H_I |\kappa, m, N\rangle = \frac{\hbar g}{2} \sqrt{N} (|\kappa, m + 1, N\rangle + |\kappa, m - 1, N\rangle), \ N = 0, 1, 2, \ldots \tag{2.78}$$

As for the dressed states in the Jaynes Cummings model, states with different excitation number $N$ do not couple. As a result, the Schrödinger equation can be solved independently for each excitation number $N$, for which the problem is equivalent to the classical field problem discussed in section 2.2 with $R$ replaced by $g\sqrt{N}$. Furthermore, equation (2.78) shows that the states with $N = 0$ do not participate in the interaction. They are states describing an atom in the ground state in an empty cavity (the vacuum), represented by
As in the semiclassical situation of Eq. (2.38), we can for fixed $\kappa$ and $N$ expand every eigenstate $|\phi_{\nu,N}(\kappa)\rangle$ in a Fourier series

$$|\phi_{\nu,N}(\kappa)\rangle = \sum_m \chi_{m,\nu,N}(\kappa)|\kappa,m,N\rangle,$$

(2.79)

so that in terms of the expansion coefficients $\chi_{m,\nu,N}$ the Schrödinger equation (2.65) reads

$$\left[ E_{\nu,N}(\kappa) - E_m^{(0)}(\kappa) \right] \chi_{m,\nu,N}(\kappa) - \frac{\hbar g}{2} \sqrt{N} \left( \chi_{m-1,\nu,N}(\kappa) + \chi_{m+1,\nu,N}(\kappa) \right) = 0,$$

$$N = 0, 1, 2, \ldots$$

(2.80)

### 2.3.2 Time Evolution

The time evolution of the state vector is given by

$$|\psi(t + \Delta t)\rangle = U |\psi(t)\rangle,$$

(2.81)

where $U = e^{-i\hat{H}\Delta t}$. We use the eigenfunctions $|\phi_{\nu,N}(\kappa)\rangle$ of $H_Q$ to expand $U$ as

$$U = \int_{-\pi}^{\pi} d\kappa \sum_{\nu,N} e^{-i E_{\nu,N}(\kappa)\Delta t} |\phi_{\nu,N}(\kappa)\rangle \langle \phi_{\nu,N}(\kappa)|.$$

(2.82)
In the bare state basis, the matrix elements of $U$ assume the form

$$\langle \kappa, m, N | U | \kappa', m', N' \rangle = \delta(\kappa - \kappa') \delta_{N,N'} U_{m,m'}(\kappa, N) \tag{2.83}$$

with

$$U_{m,m'}(\kappa, N) = \sum_{\nu} e^{-\frac{i}{\hbar} E_{\nu}(\kappa) \Delta t} \chi_{m,\nu,N}(\kappa) \chi_{m',\nu,N}^*(\kappa). \tag{2.84}$$

This allows us to express the time evolution of the vector $|\psi\rangle$ as

$$|\psi(t + \Delta t)\rangle = \int_{-q}^{q} d\kappa \sum_{m,N} C_{m,N}(\kappa, t + \Delta t) |\kappa, m, N\rangle, \tag{2.85}$$

where

$$C_{m,N}(\kappa, t + \Delta t) = \sum_{m'} U_{m,m'}(\kappa, N) C_{m',N}(\kappa, t) \tag{2.86}$$

are the expansion coefficients of the wave function $|\psi(t + \Delta t)\rangle$ in terms of the electro-translational field states $|\kappa, m, N\rangle$ as a function of the equivalent expansion coefficients of $|\psi(t)\rangle$.

### 2.3.3 Momentum Statistics and Photon Statistics

In the following we assume that the initial probability amplitudes $C_{m,N}(\kappa, t_0)$ are given by

$$C_{m,N}(\kappa, t_0) = \delta_{m,m_0} \delta(\kappa - \kappa_0) \sqrt{P_{N,m_0}}. \tag{2.87}$$
i.e. the atomic momentum distribution is initially a $\delta$-function. The probability functions $P_{N,m_0}$ describe the initial photon statistics of the field mode. Specifically, if $m_0$ is even, $P_{N,m_0}$ is the probability for the Fock state $|n = N\rangle$, $N = 0, 1, 2, \ldots$, and if $m_0$ is odd, it is the probability for the Fock state $|n = N-1\rangle$, $N = 1, 2, 3, \ldots$, and 0 for $N = 0$:

$$P_{N,m_0} \equiv \begin{cases} P(n = N) & \text{if } m_0 \text{ even, } N = 0, 1, 2, \ldots, \\ P(n = N - 1) & \text{if } m_0 \text{ odd, } N = 1, 2, 3, \ldots, \\ 0 & \text{if } m_0 \text{ odd, } N = 0. \end{cases}$$ (2.88)

From (2.85), the state vector at time $t$ becomes

$$|\psi(t)\rangle = \sum_{\nu,m_0} \sqrt{P_{N,m_0}} e^{-iE_{\nu,N}(\kappa_0)(t-t_0)} \chi_{m_0,\nu,N}(\kappa_0)\chi_{m,\nu,N}(\kappa_0)|\kappa_0, m, N\rangle,$$ (2.89)

and the probability $P(p = \hbar(\kappa_0 + m_0))$ for the atom to have momentum $p = \hbar(\kappa_0 + m_0)$ at the time $\tau$ is given by

$$P(p = \hbar(\kappa_0 + m_0)) = \sum_{\nu,N} \int d\kappa P_{N,m_0}\chi_{m_0,\nu,N}(\kappa_0)|\kappa_0, m, N\rangle|^2 |\chi_{m,\nu,N}(\kappa_0)|^2$$

$$+ 2 \sum_{N,\nu > \nu'} \int d\kappa P_{N,m_0}\chi_{m_0,\nu,N}(\kappa_0)\chi_{m_0,\nu',N}(\kappa_0)\chi_{m,\nu,N}(\kappa_0)\chi_{m,\nu',N}(\kappa_0)$$

$$\times \cos\left(\frac{E_{\nu,N}(\kappa_0) - E_{\nu',N}(\kappa_0)}{\hbar}\tau\right).$$ (2.90)
Similarly, the probability \( P(n) \) to find the field in a Fock state \( |n\rangle \) after time \( \tau \) is

\[
P(n) = \sum_{m, n} \int d\kappa |\langle \kappa_0, m, N = n | \psi(\tau) \rangle|^2
\]
\[+ \sum_{m, n} \int d\kappa |\langle \kappa_0, m, N = n + 1 | \psi(\tau) \rangle|^2,
\]

which evaluates to

\[
P(n) = \sum_{\nu, m, n} \mathcal{P}_{n, m_0} |X_{m_0, \nu, n}(\kappa_0)|^2 |X_{m, \nu, n}(\kappa_0)|^2
\]
\[+ \sum_{\nu, m, n} \mathcal{P}_{n+1, m_0} |X_{m_0, \nu, n+1}(\kappa_0)|^2 |X_{m, \nu, n+1}(\kappa_0)|^2
\]
\[+ 2 \sum_{\nu > \nu', m, n} \mathcal{P}_{n, m_0} X_{m_0, \nu, n}(\kappa_0) X_{m, \nu, n}(\kappa_0) X_{m, \nu', n}(\kappa_0) \times \cos \left( \frac{E_{\nu, n}(\kappa_0) - E_{\nu', n}(\kappa_0)}{\hbar} \tau \right)
\]
\[+ 2 \sum_{\nu > \nu', m, n} \mathcal{P}_{n+1, m_0} X_{m_0, \nu, n+1}(\kappa_0) X_{m, \nu, n+1}(\kappa_0) X_{m, \nu', n+1}(\kappa_0) \times \cos \left( \frac{E_{\nu, n+1}(\kappa_0) - E_{\nu', n+1}(\kappa_0)}{\hbar} \tau \right).
\]

2.3.4 Diffraction from Various Quantum Fields

Armed with this formalism, we now discuss the effect of different initial fields on atomic diffraction. We consider a number state, a coherent field, and a thermal field as possible initial fields. The atoms are assumed to be initially in their lower electronic state, and to have a momentum \( p = 0 \).

Since we are eventually only interested in the momentum and photon statistics, we do
not have to use a density matrix approach to treat mixed states of the initial field, such as a thermal field. We can instead work with the wave function approach presented in the previous section, introducing however an additional phase factor $e^{i\zeta_N}$ in the definition of the probability amplitudes $C_{m,N}(\kappa, t_0)$ in equation (2.87). With the integration of the phases $\zeta_N$ over an appropriate distribution $P(\zeta_N)$, this form of the initial state vector amplitude allows us to treat mixed states of the initial field.

Table 2.1 gives the appropriate photon statistics $P(n)$ for different initial fields. For

<table>
<thead>
<tr>
<th>Initial Field</th>
<th>$P(n)$</th>
<th>$2^{nd}$ Moment $\langle n^2 \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fock State</td>
<td>$\delta_{m,n}$</td>
<td>$\langle n \rangle^2$</td>
</tr>
<tr>
<td>Thermal Field</td>
<td>$\frac{(n+1)^{m+1}}{n!}$</td>
<td>$\langle n \rangle + 2\langle n \rangle^2$</td>
</tr>
<tr>
<td>Coherent Field</td>
<td>$e^{-\langle n \rangle} \frac{n^m}{n!}$</td>
<td>$\langle n \rangle + \langle n \rangle^2$</td>
</tr>
</tbody>
</table>

Table 2.1: Photon statistics for different quantum fields

the Raman-Nath regime and the resonances discussed in section 2.2 it is again possible to derive analytical solutions.

**Raman Nath Regime**

By generalization of equations (2.18) and (2.19), we can write the probability to find the atom deflected with momentum $p = m\hbar q$ after an interaction time $\tau$ as:

$$P_m = \sum_n P(n)J_m^2(\sqrt{ngr})$$

(2.93)
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for \( \delta \ll \sqrt{\langle n \rangle} g \), and

\[
P_{2m} = \sum_n P(n) J_m^2 \left( \frac{ng^2}{2\delta} \right)
\]

(2.94)

for \( \delta \gg \sqrt{\langle n \rangle} g \). The restrictions on the interaction time (Eqs. (2.20) and (2.21)) translate into

\[
\tau \ll \begin{cases} 
\frac{1}{\sqrt{\langle n \rangle} \text{gw}_{\text{rec}}} & \text{for } \delta \ll \sqrt{\langle n \rangle} g, \\
\frac{\sqrt{2\text{gw}_{\text{rec}}}}{\langle n \rangle g} & \text{for } \delta \gg \sqrt{\langle n \rangle} g.
\end{cases}
\]

(2.95)

For all inequalities we have replaced the semiclassical Rabi frequency \( R \) with the mean Rabi frequency \( \sqrt{\langle n \rangle} g \). The standard deviation in the momentum acquired by the beam after time \( \tau \) is found to be (see Eqs. (2.22)-(2.24))

\[
\sqrt{\langle p^2 \rangle} \approx \begin{cases} 
\hbar g \tau \sum_n n P(n) = \hbar g \sqrt{\langle n \rangle} g \tau & \text{for } \delta \ll \sqrt{\langle n \rangle} g, \\
\hbar q^2 g^2 \tau \sum_n n^2 P(n) = \hbar q \sqrt{\langle n \rangle} g \tau & \text{for } \delta \gg \sqrt{\langle n \rangle} g.
\end{cases}
\]

(2.96)

According to this equation, fields with frequencies close to the atomic resonance frequency and with the same average photon number \( \langle n \rangle \) will produce approximately the same standard deviation \( \sqrt{\langle p^2 \rangle} \) of the atomic momentum distribution.

For \( \delta \gg \sqrt{\langle n \rangle} g \) on the other hand, the momentum spread is proportional to \( \langle n^2 \rangle \). As Table 2.1 shows, the variance \( \langle n^2 \rangle \) for a given mean photon number \( \langle n \rangle \) is different for the various fields considered, and we expect different results.

These findings are illustrated in figures 2.8 (A)—2.8 (C), which display the time evolution of the momentum distribution of an atom interacting with a standing-wave quantum
field for various initial photon statistics. In all cases the atom is initially in its lower electronic state, and has the momentum \( p = 0 \). Furthermore, the vacuum Rabi frequency \( g = 15\omega_{\text{rec}} \), the detuning \( \delta = 0 \), and the average photon number \( \langle n \rangle = 9 \). Fig. 2.8 (A) shows the evolution for an initial Fock state, Fig. 2.8 (B) for an initial coherent field, and Fig. 2.8 (B) for an initial thermal field. Fig. 2.8 (D) compares all three cases at \( \tau = 0.1/\omega_{\text{rec}} \).

The dynamics shown in figure 2.8 (A) are identical to that of an atom interacting with a classical standing-wave field of Rabi frequency \( \mathcal{R} = \sqrt{\langle n \rangle} g \), since the equations of motion are formally the same in both cases. In the Raman-Nath regime, limited by \( \tau \ll 0.9/\omega_{\text{rec}} \) (see Eq. (2.95)), we clearly observe the Bessel function solutions of equation (2.19). This explains the linear growth of the momentum variance, and the momentum distribution with maxima on which is even better visible in Fig 2.8 (D). Around \( \tau = 0.1/\omega_{\text{rec}} \), however, this linear growth stops, and the effect of the recoil-term sets in, culminating in the revival of the probability for the momentum \( p = 0 \) at \( \tau \approx 0.35/\omega_{\text{rec}} \). Note the strong oscillations visible in the center part of the figure.

Fig. 2.8 (B) for the coherent field shows features very similar to those of figure 2.8 (A), with the main difference that the strong oscillations visible in the center region of Fig 2.8 (A) are smoothed out. This smoothing is readily explained by the sum appearing in equation (2.95). In the Raman-Nath regime this leads for the probability of each momentum state to a sum over same-order Bessel functions with arguments \( \sim \sqrt{n} \), where \( n \) is the summation index. This averaging process explains also the less pronounced revival of the \( p = 0 \) state far beyond the Raman-Nath regime.
Figure 2.8: Time evolution of the momentum distribution of an atom interacting with a standing-wave quantum field for different initial photon statistics. In all cases the atom is initially in its lower state, and has momentum $p = 0$. Furthermore $g = 15$, $\delta = 0$ (in units of $\omega_{\text{rec}}$), and $\langle n \rangle = 9$. Figure (A) shows the evolution for an initial Fock state, Fig. (B) for a coherent field, and Fig. (C) for a thermal field. Fig. (D) compares the momentum distribution for these three fields after $\tau = 0.1$, which is close to the end of the domain of validity of the Raman-Nath regime.
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The behavior of the system for an initial thermal field which is displayed in figure 2.8 (C) shows major differences. The wings of figures 2.8 (A) and 2.8 (B) are replaced by a distribution with a Gaussian envelope centered at $p = 0$ (see Fig 2.8 (D)). Furthermore, there is always a substantial population of the initial $p = 0$ component due to the large probability ($\approx 0.1$ for $\langle n \rangle = 9$) to find a thermal field in the vacuum. We have seen that an atom in the ground state does not interact with this state of the field. The smoothness of the momentum distribution is as for the coherent field due to the sum over all field states.

![Figure 2.9: Root-mean-square momentum spread as a function of interaction time for the simulations displayed in figures 2.8 (A)–2.8 (C).](image)

Figure 2.9 shows the time development of the momentum variance for the simulations displayed in figures 2.8 (A)–2.8 (C). The linear increase for the Raman-Nath regime ($\tau \ll 0.1/\omega_{\text{rec}}$) is as predicted by equation (2.96).

Quantum Pendelösung - Collapse and Revivals

The quantum nature of the electromagnetic field also influences the resonances discussed in section 2.2.4. The restriction of the analysis to just one manifold $N$ permits us to derive
analytical results, since for each $N$ we can carry out the same analysis as for classical fields. We expect the performance of the Doppleron resonances to be strongly inhibited by the “granularity” of the field, since both the energy gaps which determine the frequency of oscillation, and the detuning required to make the Doppleron work depend on the photon number $n$. Hence, even though the extension of our discussion to Doppleron resonances would be straightforward, we will only discuss Bragg resonances.

For simplicity we assume the atom to be initially in its lower electronic state, so that to describe the case of quantized fields we only need to replace $\mathcal{R}$ by $\sqrt{n}g$ and sum over all $n$ in equations (2.53), with a weight given by the field photon statistics. The energy gap for Bragg resonances, $\Delta E_{n,Bragg}$, is for a given number state $|n\rangle$ given by

$$\Delta E_{n,Bragg} = 2\left(\frac{\alpha^2}{\Delta_{Bragg}}\right)^l \frac{1}{4(l-1)[(l-1)]^2},$$

and the probability for the atom to be deflected beam becomes

$$P_1(\tau) \approx \frac{1}{2} \left[ 1 - \sum_n P(n) \cos(\frac{\Delta E_{n,Bragg}}{\hbar} \tau) \right].$$

Both for a thermal field and for a coherent field, the sum appearing in equation (2.98) can be approximated by an integral which can be evaluated analytically. It is readily seen from the Jaynes-Cummings model and the two-photon Jaynes-Cummings model [53, 54], that this approximation leads to a correct description of the collapse of $P_1(\tau)$, although it fails to predict its subsequent revivals. The integral is especially easy for the case $l = 1$
which we will consider here.

For large enough \( \langle n \rangle \), the discrete Poisson distribution \( P(n) \) of a coherent field can be approximated by a continuous Gaussian

\[
P(n) \rightarrow p(x) = \frac{1}{\sqrt{2\pi \langle n \rangle}} e^{-\frac{(x-\langle n \rangle)^2}{2\langle n \rangle}}, \tag{2.99}
\]

so that

\[
P_1(\tau) \approx \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{2\pi \langle n \rangle}} \cos \left( \frac{\langle n \rangle}{2\delta} \tau \right) \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2\langle n \rangle}} \cos \left( \frac{\langle n \rangle}{2\delta} x \tau \right) \right]
\]

\[
= \frac{1}{2} \left[ 1 - \cos \left( \frac{\langle n \rangle}{2\delta} \tau \right) e^{-\frac{\langle n \rangle^2\tau^2}{4\delta^2}} \right]. \tag{2.100}
\]

In the case of a thermal field we approximate the discrete distribution (see Table 2.1) by a continuous distribution

\[
P(n) \rightarrow p(x) = \frac{1}{\langle n \rangle} e^{-x/\langle n \rangle}, \tag{2.101}
\]

so that the probability \( P_1 \) can be expressed as

\[
P_1(\tau) \approx \frac{1}{2} \left[ 1 - \frac{1}{\langle n \rangle} \int_{0}^{\infty} dx e^{-x/\langle n \rangle} \cos \left( \frac{\langle n \rangle}{2\delta} x \tau \right) \right]
\]

\[
= \frac{1}{2} \left[ 1 - \frac{1}{1 + \left( \frac{\langle n \rangle}{2\delta} \tau \right)^2} \right]. \tag{2.102}
\]

In this case, \( P_1(\tau) \) does not undergo any oscillations, but rather a smooth increase, ac-
CHAPTER 2. COHERENT INTERACTION

accompanied by a corresponding decrease of $P_0$. As for the coherent case, revivals are not predicted due to the continuous description of the photon statistics.

The approximate forms (2.100) and (2.102) predict that the collapse of $P_1(\tau)$ occurs at

$$t_{c,\text{Coh}} \approx \frac{\sqrt{8 \log 2} \delta}{g^2 \sqrt{\langle n \rangle}}$$

(2.103)

for the coherent field, and at

$$t_{c,\text{Thermal}} \approx \frac{2\delta}{g^2 \langle n \rangle}$$

(2.104)

for the thermal field. It is important to remark that the collapse we predicted for the coherent field could also be induced by normally distributed fluctuations in the field intensity of the classical field we dealt with in previous sections [46].

We turn now to the discussion of some numerical simulations which take the whole set of equations (2.80) into account. In all simulations, the atom is initially in its lower electronic state, and has a momentum $p = \hbar q$. The dipole coupling constant $g = 15\omega_{\text{rec}}$, and the average photon number $\langle n \rangle = 9$. For the first set of simulations the detuning $\delta = 2000\omega_{\text{rec}}$, so that according to equation (2.95) the conditions for a Bragg resonance are very well fulfilled. For the second set the detuning was chosen to be $\delta = 200\omega_{\text{rec}}$, so that we expect a decrease in quality of the resonances compared to the results of the first set.

Figures 2.10 (A) and 2.10 (B) show the results of two simulations for an initial Fock state. As expected, for $\delta = 2000\omega_{\text{rec}}$ (Fig. 2.10 (A)) the Bragg resonance is very clean, and the probabilities for $p = \hbar q$ and $p = -\hbar q$ show perfect sinusoidal oscillations. No
Figure 2.10: Quantum Pendelösung for an initial Fock state of the field. The atom is initially in its lower electronic state and has momentum $p = \hbar q$. For (A) $\delta = 500$, for (B) $\delta = 200$, and for both $g = 15$ and $\langle n \rangle = 9$ (in recoil units).

side-modes are excited. Figure 2.10 (B) for $\delta = 200\omega_{\text{rec}}$ still shows nice oscillations, but the transfer between the states of momenta $p = \hbar q$ and $p = -\hbar q$ is only about 80% to 90%, and side modes are significantly excited. We would expect the same results from a classical field with $\mathcal{R} = g\sqrt{\langle n \rangle}$.

Figures 2.11 (A) and 2.11 (B) display the equivalent simulations for an initial coherent state of the field. As predicted by Eqn. (2.103) they show collapses at $\tau \approx 7/\omega_{\text{rec}}$ and $\tau \approx 0.7/\omega_{\text{rec}}$ (half the maximal amplitude). From equations (2.100) and (2.103) we can infer that the number of oscillations in the collapse time for an initial coherent field,

$$N.O.(t_{\text{c,Coh}}) \approx \frac{8\log 2\langle n \rangle}{2\pi}, \quad (2.105)$$
Figure 2.11: Quantum Pendellösung for an initial coherent state of the field. The atom is initially in its lower electronic state and has momentum \( p = \hbar q \). For (A) \( \delta = 2000 \), for (B) \( \delta = 200 \), and for both \( g = 15 \) and \( \langle n \rangle = 9 \) (in recoil units).

Figure 2.12: Quantum Pendellösung for an initial thermal state of the field. The atom is initially in its lower electronic state and has momentum \( p = \hbar q \). For (A) \( \delta = 2000 \), for (B) \( \delta = 200 \), and for both \( g = 15 \) and \( \langle n \rangle = 9 \) (in recoil units).
depends only on the average photon number and remains constant for the results displayed. The expected revivals due to the granular nature of the field are visible in both figures, and are of nearly perfect nature. However, the character of these revivals changes as we go from the larger detuning in figure 2.11 (A) to the smaller detuning in figure 2.11 (B). In figure 2.11 (A) the revivals are quasi-periodic, while they become aperiodic for the smaller detunings of figure 2.11 (B). This transition from periodic to aperiodic behavior is due to the fact that for small detunings the field induces real transitions in the atom. In that case the $\sqrt{n}$-character of the "one-photon" Rabi transition, rather than the $n$-character of the "two-photon" Rabi frequency becomes dominant. And it is this $n$-character of the "two-photon" Rabi frequency that leads to an argument proportional to $n$ in equation (2.98) for the first order Bragg resonance, and is responsible for periodic revivals. Note that this is no longer true for higher ($l^{th}$)-order Bragg-resonances, which lead to arguments $\sim n^l$ (see Eqn. (2.97)). For them we do not expect periodic revivals.

The time evolution for an initial thermal field is displayed in figures 2.12 (A) and 2.12 (B). As predicted by equation (2.104) the collapse occurs at $\tau \approx 2/\omega_{\text{rec}}$ and $\tau \approx 2/\omega_{\text{rec}}$, respectively. Furthermore, in strong contrast to the evolution for the initial coherent field, the probabilities for $p = hq$ and $p = -hq$ do not oscillate before the collapse. This is in strong agreement with equation (2.102). Note also, that the first revival visible in Fig. 2.12 does not exhibit any oscillations either.
CHAPTER 3

SPONTANEOUS EMISSION

In this chapter we add to the coherent interaction of the atomic beam with the laser field described by the Hamiltonian (2.1) the incoherent effects of spontaneous emission, so that our total system is now comprised of the two-level atom, the light field and a reservoir. The coupling between the different components is schematically shown in Fig. 3.1. As before we have the coherent coupling between the laser field and the atom. In addition, we also have the coupling of the atom to a reservoir, which we assume to be comprised of all modes of the quantum vacuum field.

Figure 3.1: System schematic for the scattering problem including spontaneous emission
3.1 The Generalized Optical Bloch Equations

The complete dynamics of the atom inside the laser-beam is described by a Liouville-von-Neuman equation for the atomic density matrix $\rho$ which takes into account the recoil effect associated with both induced and spontaneous transitions [55]

$$\dot{\rho} = \left( L_{H(t)} + L_D \right) \rho, \quad (3.1)$$

where

$$L_{H(t)} \rho = -\frac{i}{\hbar} [H(t), \rho] \quad (3.2)$$

describes the reversible part of the atom-laser interaction, while the term $L_D \rho$ accounts for spontaneous emission. Assuming the same geometry as in chapter 2, the Hamiltonian $H(t)$ is given again by equation (2.1),

$$H(t) = \frac{\vec{p}^2}{2M} - \hbar \delta |e\rangle \langle e| + \hbar R f(t) \cos qx (\sigma_+ + \sigma_-), \quad (3.3)$$

where for generality we have explicitly written down the time dependence. The irreversible part $L_D \rho$ of Eq. (3.1) is described by [55]

$$L_D \rho = -\frac{\Gamma}{2} (\sigma_+ \sigma_- \rho + \rho \sigma_+ \sigma_-) + \Gamma \int d^2 \Phi(n) e^{-i q \vec{r} \cdot \vec{n}} \sigma_- \rho \sigma_+ e^{i q \vec{r} \cdot \vec{n}}. \quad (3.4)$$
A detailed derivation of this equation is given in Appendix A. For our purposes at this point, we only remark that $\Gamma$ is the rate of spontaneous emission, and

$$\Phi(n)d^2n = \frac{3}{8\pi} \left[ \frac{1 - \left(\mathbf{p} \cdot \mathbf{n}\right)^2}{\mathbf{p}^2} \right] d^2n \quad (3.5)$$

is the probability of spontaneous emission into a solid angle $d^2n$ in the $\mathbf{n}$ direction. The exponentials in Eq. (3.4) account for the atomic recoil associated with a spontaneous emission event, and $\mathbf{r}$ is the position operator of the atom. We assume linear polarized laser light. Eqs. (3.1)–(3.5) are commonly referred to as the generalized optical Bloch equations (GOBE).

### 3.2 The Solution of the GOBE

A great deal of effort has been invested in the past to derive equations which are somewhat more transparent than the GOBE [56, 57], and to obtain approximate solutions.

The most popular approximation is the Raman-Nath approximation discussed in section 2.1.1, in which the kinetic energy operator of the Hamiltonian (3.3) is neglected [57]. The resulting differential equations are effectively of first order, and have been studied by several authors [55]. Two sub-regimes have been particularly successfully investigated: The purely diffractive regime, in which the average number of spontaneous emissions [57]

$$\bar{N} \approx \frac{R^2}{4\beta^2 + \Gamma^2 + 2R^2\Gamma \tau} \quad (3.6)$$
during the interaction time $\tau$ is much smaller than one, $\bar{N} \ll 1$, and the purely diffusive regime, in which spontaneous emission dominates, i.e. $\bar{N} \gg 1$. In the purely diffractive regime all the results from chapter 2 hold, while in the purely diffusive regime a Fokker-Planck-type equation can be derived for the time evolution of the spread in atomic momentum [57]. However, no predictions were so far possible about the experimentally important intermediate regime with $\bar{N} \sim 1$ [31].

For the resonances discussed in section 2.2.4 the Raman-Nath approximation is not valid, and different approaches had been chosen for their complete description. For good Bragg resonances with $\delta \gg \omega_{\text{rec}}$ no inclusion of spontaneous emission is necessary, and the coherent treatment of chapter 2 is sufficient. This is because the detuning $\delta$ between the atomic transition frequency and the laser frequency is so large, that the upper electronic level is never populated if the atom is initially in the ground state, and spontaneous emission is negligible. This argument holds of course not for Doppleron resonances, which always involve both atomic levels (see section 2.2.4). For them, a semiclassical force description had been developed for the strong field limit, taking into account the effects of spontaneous emission [48, 49].

In the following we discuss a method of numerical solution that makes numerical simulations possible in all regimes [58, 59]. Tan and Walls have also recently developed a numerical procedure to integrate the GOBE [60]. However, being mainly interested in the simulation of a series of experiments recently performed at MIT [31], they invoked again the Raman-Nath approximation to reduce the numerical complexity of a brute-force integration
of the GOBE. By contrast, the integration scheme described below is not limited to the Raman-Nath regime or by any other approximation.

Iterative Numerical Solution

Given the density operator at time \( t \), the formal solution of Eq. (3.1) at a later time \( t + \Delta t \) may be written

\[
\rho(t + \Delta t) = T \left\{ e^{\int_t^{t+\Delta t} dt' (H(t') + L_D)} \right\} \rho(t),
\]

(3.7)

where \( T \) indicates positive time ordering. For \( \Delta t \) small enough for \( H(t) \) to remain practically constant during the evolution from \( t \) to \( t + \Delta t \) (and in particular throughout our beam profile (2.2)), this solution can be approximated by

\[
\rho(t + \Delta t) \approx e^{(H(t) + L_D)\Delta t} \rho(t).
\]

(3.8)

In the spirit of the Lie-Trotter product formula [61, 62], which allows to disentangle the exponential for infinitesimally small time steps \( \Delta t \), we obtain

\[
\rho(t + \Delta t) = e^{L(t)\Delta t} e^{L_D\Delta t} \rho(t),
\]

(3.9)

where commutators of order \( \Delta t^2 \) have been neglected in the exponents. In practice, the solution (3.9) is valid provided that \( \Delta t \) is smaller than any relevant time scale inherent in the Hamiltonian and the dissipative evolution.
Motivated by the product form of Eq. (3.9), we write the numerical solution of the GOBE (3.1) as a two-step iteration routine in which the density operator is alternately propagat ed by the irreversible and by the reversible evolution operators,

\[
\rho(t) \rightarrow \tilde{\rho} \equiv e^{L_D \Delta t} \rho(t),
\]

\[
\tilde{\rho} \rightarrow \rho(t + \Delta t) = e^{L_H(t) \Delta t} \tilde{\rho} \equiv U \tilde{\rho} U^\dagger,
\]

where the unitary operator \( U = e^{\frac{i}{\hbar} H(t) \Delta t} \).

An advantage of the procedure (3.10), compared to, say, a Runge-Kutta algorithm, is that it is strictly norm-conserving even if the physical situation allows for a large step size \( \Delta t \) \[63\]. In fact, the formula (3.9) is exact for both the cases \( \Gamma = 0, H(t) = \text{const.} \), and \( H(t) = 0, \Gamma \neq 0 \), which provide useful checks of the numerical routine. Moreover, this procedure requires the simultaneous storage of only two density matrices. By contrast, a fourth-order Runge-Kutta algorithm requires even without variable step size the simultaneous storage of at least three different density matrices.

We are left with the task of finding practical implementations for the two steps in equation (3.10).

**The Irreversible Part**

The irreversible evolution is readily obtained by solving the GOBE with \( H(t) \) set equal to zero. Being interested in the atom dynamics along the laser-axis (the x-axis), we assume the
y- and z-components of the atomic position operator to commute with $\rho$. For the "initial" density matrix $\rho(t)$ expressed in momentum representation as

$$\rho_{\alpha\beta}(p,p') = \langle p, \alpha | \rho | p', \beta \rangle$$

(3.11)

where $p$ is the atomic momentum in the $x$-direction, and $\alpha, \beta$ label the electronic state of the atom, the solution of the irreversible evolution may be expressed as

$$\tilde{\rho}_{ee}(p,p') = \rho_{ee}(p,p';t)e^{-\Gamma \Delta t},$$

$$\tilde{\rho}_{eg}(p,p') = \rho_{eg}(p,p';t)e^{-\Gamma \Delta t/2},$$

$$\tilde{\rho}_{gg}(p,p') = \rho_{gg}(p,p';t) + \left[1 - e^{-\Gamma \Delta t}\right] \int_{-1}^{1} d\eta \omega(\eta) \rho_{ee}(p + \hbar \eta, p' + \hbar \eta).$$

(3.12)

Here $w(\eta)d\eta$ is the probability for the spontaneous emission to occur in a direction $\mathbf{n}$ with $x$-component $\eta$,

$$w(\eta) = \int d^2 \Phi(\mathbf{n}) \delta(n_x - \eta),$$

(3.13)

and $\Phi(\mathbf{n})$ is the dipole characteristic of the atomic spontaneous emission pattern given in Eq. (3.5).

The Hamiltonian Part

Eq. (3.10) shows that we need a suitable matrix representation of the unitary operator $U = \exp(-iH\Delta t/\hbar)$ in order to implement the Hamiltonian part (we limit our discussion
here again to the profile function (2.2) so that the Hamiltonian is constant). The band theoretical approach of section 2.2 provides in equations (2.42)-(2.44) a representation of \( U \),

\[
U_{m,m'}(\kappa) = \sum_{\nu} e^{-i \frac{\hbar}{\Delta t} E_{\nu}(\kappa)} \chi_{m\nu}(\kappa) \chi_{m'\nu}(\kappa),
\]

which is very suitable for this purpose. The coefficients \( \chi_{m\nu}(\kappa) \) and the energies \( E_{\nu}(\kappa) \) are determined by the solution of the tridiagonal eigenvalue problem (2.40), which is in turn easily solved by choosing appropriate cutoffs of equations (2.40).

With equation (3.14), the evolution of the Hamiltonian phase of equation (3.10) is given by

\[
\rho_{m,m'}(\kappa, \kappa'; t + \Delta t) = \sum_{i,i'} U_{m,i}(\kappa) \tilde{\rho}_{i,i'}(\kappa, \kappa') U_{i,m'}^{*}(\kappa'),
\]

and is thereby reduced to a simple matrix multiplication for each pair \( \kappa, \kappa' \) of quasi wave numbers.

What remains to be done is to re-express equations (3.12) for the irreversible evolution in terms of the \( \kappa, m \) representation, and to chose a suitable discretization of the continuous wavenumber \( \kappa \). The first task is achieved without difficulty by writing the \( p \) arguments of Eqs. (3.12) as \( p = \hbar(\kappa + m)q \) where \( -q \leq \kappa < q \) (first Brillouin zone) and \( m \) is an integer, and by associating even \( m \)'s (odd \( m \)'s) with the lower (upper) electronic state of the atom. The task of finding a suitable discretization is dictated by physical circumstances. For most cases, the discretization \( \Delta \kappa = q/4 \) proved to be sufficient. More details on the implementation and the choice of the time step \( \Delta t \) are given in Appendix B.
3.3 Transition from the Diffractive to the Diffusive Regime

In this section we investigate the transition from the diffractive to the diffusive regime, characterized by a change of the number of spontaneously emitted photons $\bar{N}$ (see Eq. (3.6)) from zero for the purely diffractive regime to a value much larger than one for the purely diffusive regime. We consider first the symmetric momentum spread of an atomic beam entering the interaction region with a transverse momentum $p = 0$. The impact of spontaneous emission on two-beam resonances is the subject of section 3.4.

3.3.1 Raman-Nath Regime

Gould et al. [31] recently published results of a sodium-beam experiment aimed at investigating the transition between the diffractive and diffusive regimes. All experiments were performed under conditions where the Raman-Nath approximation holds, the interaction time $\tau = 0.015/\omega_{\text{rec}}$ being in all cases at most half the upper value given by conditions (2.20) and (2.21). The variation of $\bar{N}$ was mainly achieved by changing the detuning $\delta$, thereby changing the population of the upper state. We will use the experimental results as the basis for our discussion.

Our numerical simulations and the experiments of Gould et al. are compared in Figures (3.2)—(3.4). Since we used a rectangular laser-beam profile for the simulations rather than a Gaussian profile, we compensated for this difference by appropriate slight changes in the parameters, as suggested by Tan and Walls [60]. Figures (3.2) and (3.3) display non-resonant situations with $\delta = 3200\omega_{\text{rec}}, \mathcal{R} = 1237\omega_{\text{rec}}$ and $\delta = 1600\omega_{\text{rec}}, \mathcal{R} = 1310\omega_{\text{rec}}$, respectively.
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Figure 3.2: Final momentum distribution for an atomic beam with initially Gaussian momentum distribution (centered at $p = 0$, width $\Delta p = 1.2$ (FWHM)) after the interaction with a standing light field. Here $R = 1237$, $\delta = 3200$, $\Gamma = 400$, and $\tau = .015$ (in recoil units). The corresponding experimental data ([31]) is displayed with a dashed line.

Figure 3.3: Final momentum distribution for an atomic beam with initially Gaussian momentum distribution (centered at $p = 0$, width $\Delta p = 1.2$ (FWHM)) after the interaction with a standing light field. Here $R = 1310$, $\delta = 1600$, $\Gamma = 400$, and $\tau = .015$ (in recoil units). The corresponding experimental data (see [31]) is displayed with a dashed line.
Figure 3.4: Final momentum distribution for an atomic beam with initially Gaussian momentum distribution (centered at $p = 0$, width $\Delta p = 1.2$ (FWHM)) after the interaction with a standing light field. $R = 944$, $\delta = 0$, $\Gamma = 400$, and $\tau = .015$ (in recoil units). The corresponding experimental data (see [31]) is displayed with a dashed line.

respectively. The resonant case with $\delta = 0$, $R = 944\omega_{\text{rec}}$ is shown in figure (3.4). In all cases the spontaneous emission rate is $\gamma = 400\omega_{\text{rec}}$ and the incoming atom is in its lower electronic state. The momentum distribution of the incoming atoms is taken to be a Gaussian centered at $p = 0$ with width $\Delta p = 1.2\hbar q$ (FWHM). The results demonstrate the transition from the diffractive regime (Fig. 3.2, $\tilde{N} \approx 0.4$) to the diffusive regime (Fig. 3.4, $\tilde{N} \approx 4.5$).

The agreement between the experimental data and our simulations is excellent, although the center peak in the experimental data is somewhat higher than displayed in the simulation results. This discrepancy is attributed to a non-perfect preparation of the atoms in the experiments. We also note a perfect agreement between our results and the numerical
simulations of Tan and Walls [60], which were performed using the Raman-Nath approximation. This is of course expected, since the parameters of the simulations are well inside the range of validity of the Raman-Nath approximation.

### 3.3.2 Beyond the Raman-Nath Regime

We already mentioned that a particular feature of the numerical scheme presented here is that it is not restricted to the Raman-Nath regime. To demonstrate the difference between the solution obtained with the Raman-Nath approximation and the solution obtained by fully accounting for the kinetic term of the Hamiltonian (3.3), we now compare simulations made for both cases with experimentally reachable parameters. Figure 3.5 shows the result of the exact simulations, while figure 3.6 shows the result for the simulation made under the Raman-Nath approximation. In both cases the Rabi frequency is $\mathcal{R} = 150\omega_{rec}$, the detuning $\delta = 600\omega_{rec}$, the spontaneous decay rate $\Gamma = 400\omega_{rec}$, and the maximum interaction time $\tau_{max} = a/\omega_{rec}$. Choosing the transition $3^2S_{1/2}, F = 2, m_F = 2 \leftrightarrow 3^2P_{3/2}, F' = 3, m_{F'} = 3$ in Sodium as an example, we have $\omega_{rec}/2\pi = 25$KHZ, $\Gamma/2\pi = 10$MHz, $\delta/2\pi = 15$MHz, $\tau_{\text{max}} = 2.5 \times 10^{-6}$sec and a laser power of approximately $360\mu$W, where we have used conversion factors published by Gould et al. [32]. The initial atomic momentum distribution is a Gaussian, centered at $p = 0$ with $\Delta p = 1.2\hbar q$ (FWHM). The simulations were again made for a rectangular laser beam profile. From Eq. 2.21, we find that for this set of parameters the Raman-Nath approximation holds for $\tau < 0.23/\omega_{rec}$.

The effect of the kinetic energy term on the momentum spread for $\tau > 0.1\omega_{rec}$ is clearly
Figure 3.5: Time evolution of the momentum profile of an atom beam interacting with a standing light field. The atoms are initially in the lower electronic state and have a Gaussian momentum distribution (centered at $p = 0$, width $\Delta p = 1.2$ (FWHM)). $\mathcal{R} = 150$, $\delta = 600$, $\Gamma = 400$ and $\tau_{\text{max}} = 0.4$ (in recoil units). The corresponding laser power is about $300\mu W$ and the detuning about $15\text{MHz}$. The inset shows the momentum distribution for $\tau = 0.4$ on the same scale as the inset of figure (3.5.eps).

seen by comparing figures 3.5 and 3.6. The linear growth of the momentum distribution characteristic of the Raman-Nath regime abruptly stops beyond $\tau = 0.1/\omega_{\text{rec}}$, after which time the scattering profiles of figure 7 and 8 differ substantially. Note in particular the revival of the $p = 0$ component, an effect that definitely can not be reproduced in the Raman Nath approximation.
3.4 Effects of Spontaneous Emission on Two-Beam Resonances

We already speculated that Doppleron and Bragg resonances are affected quite differently by spontaneous emission. In the following we provide evidence for this reasoning. We also learn that the impact of spontaneous emission strongly depends on the electronic state of the incoming atom, on the order $l$ of the resonance, and the initial momentum $m_0 \hbar q$. 

Figure 3.6: Time evolution of the momentum profile of an atom beam interacting with a standing light field using the same parameters as for figure 3.5, but making the Raman-Nath approximation. The inset shows the momentum distribution for $\tau = A/\omega_{rec}$ on the same scale as the inset of figure 3.5.
3.4.1 Bragg Resonances

As discussed in section 2.2.4, the GOBE for $\Gamma = 0$ are symmetric with respect to an interchange of the electronic levels and the change of sign of the detuning. This symmetry is broken if spontaneous emission is taken into account. Bragg resonances which utilize ground-state atoms remain virtually unaffected, while they are rapidly destroyed if the atom is initially excited. Figures 3.7 (A) and 3.7 (B) illustrate this behavior. They display the dynamical behavior of a Bragg resonance for an atom initially in the ground state (3.7 (A)) and in the upper state (3.7 (B)). Except for the spontaneous emission rate $\Gamma = 400\omega_{\text{rec}}$ the parameters chosen for the simulations are the same as in Fig. 2.5, i.e. $R = 385\omega_{\text{rec}}$, $\delta = 32000\omega_{\text{rec}}$. The transverse momentum of the incoming atoms is $p_0 = \hbar q$.

Figure 3.7 (A) is virtually the same as Fig 2.5, illustrating clearly that the atom remains mainly in the lower state during the interaction, thus prohibiting spontaneous emission to occur.

Figure 3.7 (B), on the other hand, is dramatically different. A spontaneous emission event occurs right at the beginning of the time evolution. This is a transient phenomenon with a characteristic time scale of $1/\Gamma = 0.025/\omega_{\text{rec}}$, which is much shorter than any time scale associated with (coherent) diffractive processes. The random recoil associated with this spontaneous emission event leads for short times to the double-peaked momentum distribution visible in the insert of Fig. (2.8 (B)). The two peaks are the result of a projection of the dipole radiation pattern on the laser-axis, as expressed in equation (3.5).

After the first spontaneous emission event, the atom is in its ground state, where it
Figure 3.7: Pendellösung effect with the same parameters as for figure 2.5, but with the inclusion of spontaneous emission with $\Gamma = 400$. For (A) the atom was initially in its lower state, and there is no visible difference to Fig 2.5. For (B) the atom was initially in its upper state. Note the immediate decay into the lower state. Note also that the interaction remains diffractive, because due to the large detuning the atom remains after the initial decay mainly in the lower state, prohibiting further spontaneous emissions to occur. The inset in (B) shows the same plot from a viewpoint in the vicinity of the positive time axis.

remains for all times to an excellent degree of approximation. Its further evolution could be obtained just as well by neglecting spontaneous emission altogether and taking the double-peaked distribution as an initial condition. It is essentially reversible and characterized by the well-defined oscillations appearing in Fig. 3.7 (B).
3.4.2 Doppleron Resonances

Doppleron resonances always involve both electronic levels, making them naturally sensitive to spontaneous emission. Compared to Bragg resonances, for which one electronic level can be effectively eliminated in the description of the coherent evolution, we expect a weak dependence on the initial state of the atom. Much more important will be the ratio of the beam splitting time $\tau_{\text{split}}$ and the spontaneous decay time $1/\Gamma$. If the splitting time $\tau_{\text{split}}$ is of the order of or smaller than $1/\Gamma$, we expect only a limited disturbance from spontaneous emission. On the other hand, if $\tau_{\text{split}} \gg 1/\Gamma$, we expect the resonance to be destroyed.

Figures 3.8 (A) and 3.8 (B) display the second-order Doppleron resonance of Fig. 2.6 with the inclusion of spontaneous emission. For both figures $\mathcal{R} = 4000\omega_{\text{rec}}$ and $p_0 = 660\hbar q$ and $p_1 = 665\hbar q$. In figure 3.8 (A) the atom is initially in the lower electronic state, and $\delta = 3640.45\omega_{\text{rec}}$, while in figure 3.8 (B) the atom is initially in its upper electronic state, and $\delta = -3640.45\omega_{\text{rec}}$. In both cases we observe the destruction of the spatial atomic coherence, and the transition from the diffractive to the diffusive regime of scattering in a time $\tau \approx 0.015/\omega_{\text{rec}}$. This is the average time after which the first spontaneous emission process occurs, not counting the initial transient. This time is of the same order as the transfer time $2\tau_{\text{split}} \approx 0.009/\omega_{\text{rec}}$ which explains that just one (coherent) transfer occurs before the resonance is washed out by spontaneous emission. The similarity of time scales for coherent and incoherent processes explains why there is no striking difference in the scattering profiles for atoms initially in the upper state or in the lower state. Note that we had to chose a negative detuning for Fig 3.8 (B), in order to achieve the same momentum
Figure 3.8: Second-order Doppleron resonance with parameters equivalent to the parameters for figure 2.6, but with the inclusion of spontaneous emission ($\Gamma = 400$). In (A) the atom is initially in the lower electronic state and $\delta = 3640.45$, in (B) the atom is initially in the upper electronic state and $\delta = -3640.45$. Due to the short transfer time of the resonance, it is still visible. Except for the cooling instead of the heating of the atomic momentum due to the different sign of the detuning, there is hardly any difference between (A) and (B). It can be clearly seen, that the systems are already in the diffusive regime at the maximum interaction time shown.

transfer as for Fig 3.8 (A) since the initial electronic levels were different. This lead to a cooling of the overall momentum in Fig 3.8 (B) in contrast to the heating visible in Fig 3.8 (A) (this heating/cooling effect is better visible in Figs. 3.9 (A) and 3.9 (B)).

In figure 2.7 of section 1.2.4 we also presented the coherent evolution of a cleaner Doppleron resonance. Figures 3.9 (A) and 3.9 (B) show the equivalent simulations with the inclusion of spontaneous emission ($\Gamma = 400\omega_{\text{rec}}$), and with the atom initially in its lower and upper electronic state, respectively. Here we did not switch the detuning for
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Figure 3.9: Improved second order Doppleron. Except for the spontaneous emission ($\Gamma = 400\omega_{rec}$) and the initial electronic state of the atom (lower in (A), and upper in (B)), the parameters are the same as for figure 2.7. Due to the long transfer time no resonance is visible anymore, and the systems are way in the diffusive regime at the largest times shown.

(A)

(B)

the simulation with the atom initially in its upper state, and both figures show clearly the heating effect on the momentum distribution. The rapid initial decay in figure 3.9 (B) is due to a single spontaneous emission event that occurs in the transient phase before the coherent interaction with the laser beam has a chance to change the internal state of the atom. As in the case of Bragg resonances, this transient effect leads for short times to a double-peaked momentum distribution. The absence of this transient in figure 3.9 (A) is a simple consequence of the fact that the atom enters the interaction region already in the ground state. The rather slow and smooth decay visible in both figures is a consequence of
spontaneous decay in the stationary regime. The time scale of this decay is given by the transfer time $2r_{split}$ of the coherent interaction. Coherences can however not build up, as spontaneous emission prevents the transfer of a significant population between levels.
CHAPTER 4

CONCLUSION

We have studied analytically and numerically the diffraction of atoms by a standing-wave light field. To do this we used a band-theoretical framework, which allows an integrated treatment of the problem.

We have explored the effects that various initial quantum fields have on the dynamics of the interaction. We have observed a smoothing of the momentum dynamics close to resonance, and the Quantum Pendellösung effect in the Bragg-resonance regime. In all regimes we noticed a strong dependence of atomic diffraction on the initial field.

We devoted special attention to the study of spontaneous emission. We characterized analytically and investigated numerically by using a split-operator technique three regimes of practical interest.

In or near the Raman-Nath regime of diffraction, the major effect of spontaneous emission is a transition from a diffraction-dominated to a diffusion-dominated regime. In the case of two-beam Bragg scattering, it has negligible effects provided the incident atoms are in their lower electronic state and the atom-field detuning is sufficiently large to guar-
antee that the upper level is never significantly populated. Finally, two-beam scattering using Doppleron resonances is typically strongly affected by spontaneous emission, as these resonances involve both the ground and the excited electronic level.
APPENDIX A

DERIVATION OF THE
MASTER EQUATION

In this appendix we derive the effective master equation for a two-level atom undergoing spontaneous emissions, explicitly taking into account the translational degree of freedom of the atom. In our model, the spontaneous emissions are caused by the coupling of the atom to a reservoir of free space modes, and the effective master equation for the atom is obtained by adiabatically eliminating the modes of the reservoir. Our derivation follows the method presented by Haake et al. in [64].

The basic Hamiltonian of the total atom–reservoir system is

\[ H = \frac{\hat{p}^2}{2M} + \hbar \omega | \xi \rangle \langle \xi | \]
\[ + \sum_j \hbar \Omega_j a_j^\dagger a_j + \sum_j (\hbar g_j \sigma_+ a_j e^{i\xi} + \hbar g^*_j \sigma_- a_j^\dagger e^{-i\xi}). \tag{A.1} \]

The atom is described by the atomic momentum operator \( \hat{p} \), the canonical conjugate po-
APPENDIX A. DERIVATION OF THE MASTER EQUATION

sition operator $\hat{F}$, and the atomic transition frequency $\omega$. The quantized modes $j$ of the reservoir are characterized by mode frequencies $\Omega_j$, wave vectors $\mathbf{q}_j$, and annihilation and creation operators $a_j$ and $a_j^\dagger$. The constants $g_j$ describe the coupling between the atom and field modes $j$, and $\sigma_+$ and $\sigma_-$ are the usual Pauli spin operators acting on the atomic ground state $|g\rangle$ and excited state $|e\rangle$.

In an interaction picture defined by the unitary transformation

$$U = e^{-i(\Omega_j)(e_{j\uparrow} + \sum_j \Omega_j a_j^\dagger a_j)t}$$  \hspace{1cm} (A.2)$$

and under the rotating wave approximation (RWA), the interaction Hamiltonian becomes

$$H_i = H_0 + H_{0B}. \hspace{1cm} (A.3)$$

Here

$$H_0 = \frac{\hat{p}^2}{2M} \hspace{1cm} (A.4)$$

gives the free evolution of the atom, and

$$H_{0B} = \sum_j (\hbar g_j \sigma_+ a_j e^{i\mathbf{q}_j \cdot \mathbf{r}} e^{i(\omega - \Omega_j)t} + \hbar g_j^* \sigma_- a_j^\dagger e^{-i\mathbf{q}_j \cdot \mathbf{r}} e^{-i(\omega - \Omega_j)t}) \hspace{1cm} (A.5)$$

describes the interaction of the atom with the reservoir, which leads to spontaneous emission.
This interaction Hamiltonian can more generally be written as

$$ H_{0B} = \sum_j (A_j B_j + A_j^\dagger B_j^\dagger) $$  \hspace{1cm} (A.6)

where the $A_j$'s are atomic operators and the $B_j$'s are reservoir operators. In our example we include the explicit time dependence into the atomic operator, so that

$$ A_j = \hbar g_j \sigma^j e^{i\mathbf{q}_j \cdot \mathbf{r} e^{-i(\omega-\Omega_j)t}} $$

and

$$ B_j = a_j. $$  \hspace{1cm} (A.7)

The Liouville-von Neuman equation for the density matrix $W$ of the atom–reservoir system is

$$ \dot{W}(t) = -\frac{i}{\hbar} W(t) \equiv L W(t) $$  \hspace{1cm} (A.8)

where the Liouville operator $L = L_0 + L_{0B}$. The formal solution of Eq. (A.8) is

$$ W(t) = e^{Lt} W(0). $$  \hspace{1cm} (A.9)

We seek an equation for the reduced density operator of the atom

$$ \rho(t) = tr_B W(t) = tr_B e^{Lt} \rho_B(0) \rho_0 $$  \hspace{1cm} (A.10)

where we have made the assumption that the atom-reservoir density matrix factorizes at
t = 0, implying that there is no initial correlation between the free atomic evolution and the reservoir. Introducing

\[ U(t) \equiv \text{tr}_B \left\{ e^{Lt} \rho_B(0) \right\} \]  

we have \( \rho(t) = U(t) \rho(0) \), and, assuming that the inverse of \( U(t) \) exists as well, can write the equation of motion for \( \rho(t) \) as

\[ \dot{\rho}(t) = \dot{U} U^{-1} \rho(t) \equiv l(t) \rho(t). \]  

Here we introduced the generator of infinitesimal time translations \( l(t) \).

We would like to expand the generator \( l(t) = \dot{U} U^{-1} \) in terms of the atom-reservoir interaction \( L_{0B} \). To zeroth order we have

\[ U^{(0)} = \text{tr}_B e^{L_{0B} t} \rho_B(0) = e^{L_{0B} t} \]  

and

\[ \dot{U}^{(0)} = L_0 U^{(0)}, \]  

where we used \( \text{tr}_B e^{L_{0B} t} = e^{L_{0B} t} \text{tr}_B \). As expected, we get \( I^{(0)} = \dot{U}^{(0)} (U^{(0)})^{-1} \)

\[ I^{(0)} = L_0. \]  

To get the higher order terms, we introduce the operators \( V = e^{Lt} \) and \( \tilde{V} = e^{-L_{0B} t}V \).
From

\[ \dot{V} = L_0 e^{Lt} = L_0 e^{Lt} + L_0 e^{Lt} \]  \hspace{1cm} (A.16)

it follows that

\[ \dot{V} = e^{-L_0 t} L_0 e^{L_0 t} \dot{V} \equiv L_0 B(t) \dot{V}, \]  \hspace{1cm} (A.17)

which can be integrated to

\[ \dot{V} = T \left\{ e^{\int_0^t dt' L_0 B(t')} dt' \right\} \]  \hspace{1cm} (A.18)

where \( T \) indicates positive time ordering which has to be applied when expanding the exponential (larger times on the left side). Equations (A.13) and (A.18) together yield

\[ U = tr B e^{L_0 t} \left\{ 1 + \int_0^t dt' L_0 B(t') + \int_0^t dt' \int_0^{t'} dt'' L_0 B(t') L_0 B(t'') \cdots \right\}. \]  \hspace{1cm} (A.19)

All that is left to do is to expand \( U^{-1} \) as well. To do this, we observe that in equation (A.19) the terms \( tr B \) and \( e^{L_0 t} \) commute, and that the normalization \( tr B \rho_B(0) = 1 \) holds, so that

\[ U^{-1} = \left\{ 1 + tr B \left[ (\int_0^t dt' L_0 B(t') + \int_0^t dt' \int_0^{t'} dt'' L_0 B(t') L_0 B(t'') + \cdots) \rho_B(0) \right] \right\}^{-1} e^{-L_0 t}. \]  \hspace{1cm} (A.20)

Using \((1 + x)^{-1} = 1 - x + \cdots\), we can write \( l(t) \) as

\[ l(t) = L_0 + tr B \left\{ L_0 B e^{L_0 t} (1 + \int_0^t dt' L_0 B(t') + \cdots) \rho_B(0) \right\} \]
\[ \times \left\{ 1 - tr_B \left[ \left( \int_0^t dt'L_{0B}(t') + \cdots \right) \rho_B(0) \right] \right\}^{-1} e^{-L_0t}. \quad (A.21) \]

Since the expectation values of the reservoir operators \( a_j \) and \( a_j^\dagger \) are zero,

\[ tr_B \left\{ L_{0B} e^{L_0} \rho_B(0) \right\} = tr_B \left\{ L_{0B} \rho_B(0) \right\} e^{L_0} = 0, \quad (A.22) \]

the first order contribution vanishes, \( I^{(0)} = 0 \), and the second order contribution reduces to

\[ I^{(2)}(t) = L_0 + tr_B \left\{ L_{0B} e^{L_0t} \int_0^t dt'L_{0B}(t') \rho_B(0) \right\} e^{-L_0t}. \quad (A.23) \]

Using equation (A.17), moving the terms \( L_{0B} e^{L_0t} \) and \( e^{-L_0t} \) in equation (A.23) under the integral, making the change of variable

\[ \tau = t - t', dt' = -d\tau, \quad (A.24) \]

and taking again into account that \( \rho_B(0) \) commutes with \( e^{L_0t} \), equation (A.12) can be approximated by

\[ \dot{\rho}(t) \approx I^{(2)}(t)\rho(t) = L_0\rho(t) + tr_B \left\{ \int_0^t d\tau L_{0B}L_{0B}(-\tau)\rho_B(0)\rho(t) \right\}. \quad (A.25) \]

We note that due to (A.17) and the commutation relation \([L_0, B_j] = 0\) only the atomic
APPENDIX A. DERIVATION OF THE MASTER EQUATION

operators acquire a time dependence in \( L_{0B}(\tau) = e^{L_0 \tau} L_{0B} e^{-L_0 \tau} \). Observing that

\[
e^{L_0 \tau} L_{0B} e^{-L_0 \tau} \rho_{0}(0) \rho(t) = -\frac{i}{\hbar} [H_{0B}(\tau), \rho_{0}(0) \rho(t)] \tag{A.26}
\]

with

\[
H_{0B}(\tau) = e^{\frac{i}{\hbar} H_{0} \tau} H_{0B} e^{-\frac{i}{\hbar} H_{0} \tau} \tag{A.27}
\]

describing the time evolution of \( H_{0B} \) under the free atom Hamiltonian \( H_{0} \), the Liouville-von Neuman equation can be written as

\[
\dot{\rho}(t) \approx L_{0} \rho(t) + \frac{1}{\hbar^{2}} \int_{0}^{t} dt \sum_{j} \langle B_{j} B_{j} \rangle_{res} ([A_{j}^{\dagger}(\tau) \rho(t), A_{j}] + H.C.). \tag{A.28}
\]

In the long time limit \( t \to \infty \) this equation becomes the master equation for the reduced density matrix of the atom. The time limit is equivalent to the Markov approximation, which means that the reservoir is taken to be white noise with an infinitely short memory.

Using the Baker-Hausdorff transformation \( e^{X} e^{Y} = e^{X+Y+\frac{1}{2}[X,Y]} \), valid if \([X,[X,Y]] = [Y,[X,Y]] = 0\), we have

\[
A_{j}(\tau) = e^{\frac{i}{\hbar} H_{0} \tau} A_{j} e^{-\frac{i}{\hbar} H_{0}} = \hbar g_{j} e^{i(q_{j} \hat{P} + \frac{q_{j}^{2}}{2M})} e^{i(\omega - \Omega_{j}) \tau} \tag{A.29}
\]
Here \( \hat{p} \) and \( \hat{r} \) still are non-commuting operators, so that we are not allowed to simply group all the time dependent terms as we would like to do in order to evaluate the integral over \( \tau \), and we continue by using the momentum representation. Taking into account the assumption that the reservoir is a vacuum, implying that \( \langle a_j a_j^\dagger \rangle = \langle A_j A_j^\dagger \rangle = 1 \) and \( \langle a_j^\dagger a_j \rangle = \langle A_j^\dagger A_j \rangle = 0 \), we end up with

\[
\dot{\rho}(p, p'; t) = \langle p | L_0 \rho(t) | p' \rangle + \sum_j \int_0^\infty d\tau |g_j|^2 \left[ e^{i(\omega - \Omega_j + \frac{p q_j}{m} + \frac{\hbar q_j^2}{2m}) \tau} \sigma_+ \rho(p + \hbar q_j, p' + \hbar q_j; t) \sigma_+ + H.C. \right] - \sum_j \int_0^\infty d\tau |g_j|^2 \left[ e^{i(\omega - \Omega_j + \frac{p q_j - \hbar q_j^2}{2m}) \tau} \sigma_+ \rho(p, p'; t) + H.C. \right]. \tag{A.30}
\]

The integrals are Laplace transforms which are related to the respective Fourier transforms by the identity

\[
\int_0^\infty dt e^{i\phi t} f(t) = \frac{1}{2} f(\phi) + \frac{i}{2\pi} P \int_{-\infty}^\infty d\nu \frac{f(\nu)}{\phi - \nu}, \quad f(\phi) = \int_{-\infty}^\infty dt e^{i\phi t} f(t). \tag{A.31}
\]

Using this identity, but neglecting the principal part, which introduces merely a frequency shift (Lamb shift), we can evaluate the infinite time integral resulting in \( \delta \)-functions which reflect the energy conservation. We proceed by replacing the sums over the modes in (A.30) by integrals. However, the second one is complicated by the \( q_j \) dependence of \( \rho \). Even though the absolute value of \( q_j \) is fixed by the \( \delta \)-function resulting from the \( \tau \) integration,
the angular dependence has to be accounted for. By denoting the spontaneous emission rate of a two level atom as $\Gamma$, we can finally write the master equation as

$$\dot{\rho}(p, p'; t) = -\frac{i}{\hbar} \left[ \frac{p^2}{2M} - \frac{p'^2}{2M} \right] \rho(p, p'; t)$$

$$- \frac{\Gamma}{2} \sigma_+ \sigma_- \rho(p, p'; t)$$

$$+ \frac{3\Gamma}{16\pi} \int d^2 n \left[ 1 - \frac{(p \cdot n)^2}{\varepsilon^2} \right] \sigma_- \rho(p + \hbar q n, p' + \hbar q n; t) \sigma_+ + H.C. \quad (A.32)$$

where $n$ is a unit vector and the integral $\int d^2 n$ is a surface integral over the unit sphere, reflecting the angular distribution of spontaneous emission.
APPENDIX B

NUMERICAL IMPLEMENTATION

B.1 Incoherent Evolution

In this appendix we summarize the numerical implementation of the solution of the GOBE based on the two-step iteration (3.10). This iteration is most conveniently performed in the \((\kappa, m)\)-representation introduced in Eq. (2.31), i.e. for the matrix elements \(\rho_{mm'}(\kappa, \kappa') \equiv \langle \kappa, m|\rho|\kappa', m'\rangle\). The transformation from the \((p, \alpha)\)-representation used in Eqs. (3.12) to the \((\kappa, m)\)-representation is achieved by

\[
m = \begin{cases} 
    2 \text{Int}[(p + 1)/2], & \text{if } \alpha = g \text{ (ground state)} \\
    2 \text{Int}[p/2] + 1, & \text{if } \alpha = e \text{ (excited state)}
\end{cases} ; \quad \kappa = p - m, \tag{B.1}
\]

where \(\text{Int}(x)\) gives the greatest integer less than or equal to \(x\). In Eq. (B.1) and other equations in this appendix the momentum \(p\) and the wave vector \(\kappa\) are for notational
simplicity scaled by $\hbar q$ and $q$, respectively.

Numerically, $\kappa$ and $\eta$ (see Eq. (3.13)) is a discrete index with $\kappa, \eta = -1, -1+\Delta \kappa, \ldots, 1-\Delta \kappa$. Once discretized, $\rho$ is represented as an array with $N_\rho = (N_m N_\kappa)^2$ elements, where $N_m$ is the number of branches taken into account, and $N_\kappa = 2/\Delta \kappa$ is the number of partitions of the Brillouin zone induced by the discretization. We will comment on these numbers below.

### B.1.1 Algorithm

Each run propagates the density matrix from its initial value to its final value at time $\tau$. On intermediate stages, the momentum distribution can be read off from the diagonal elements to generate the 3-D plots from the main chapters.

At the beginning of each run, the array $\tilde{w}(\eta) \equiv [1 - \exp(-\Gamma \Delta t)]w(\eta)\Delta \kappa$ is calculated [see Eq. (3.13)] and stored for further use in the irreversible phases of the evolution. Then the Hamiltonian is diagonalized, which yields the eigenenergies $E_\nu(\kappa)$ and eigenvector coefficients $\chi_{mn}(\kappa)$, see Eq. (2.40). With these, first the elements $U_{mn}(\kappa)$ and then the array elements $M_{mnm'n'}(\kappa, \kappa') \equiv U_{mn}(\kappa)U_{nm'}(\kappa')$ are calculated [see Eq. (2.44)]. This array is then stored for further use in the Hamiltonian phase of the evolution, see Eq. (3.15).

Using the transformation (B.1) in Eqs. (3.13), the first step describing the irreversible
evolution in the two-step iteration (3.10) reads

\begin{align*}
\text{\(m, m'\) both odd:} & & \tilde{\rho}_{mm'}(\kappa, \kappa') = e^{-\Gamma \Delta t} \rho_{mm'}(\kappa, \kappa'; t) \\
\text{\(m, m'\) different parity:} & & \tilde{\rho}_{mm'}(\kappa, \kappa') = e^{-\Gamma \Delta t/2} \rho_{mm'}(\kappa, \kappa'; t) \\
\text{\(m, m'\) both even:} & & \tilde{\rho}_{mm'}(\kappa, \kappa') = \rho_{mm'}(\kappa, \kappa'; t) + S_{mm'}(\kappa, \kappa')
\end{align*}

where \(S_{mm'}(\kappa, \kappa')\) is the recoil integral in the expression for the ground state population in Eq. (3.13). In terms of a subroutine:

\begin{enumerate}
\item \(S_{mm'} = 0; \ p = m + \kappa; \ p' = m' + \kappa'\) (initialization)
\item \text{FOR } \eta = \text{\(-1\ TO \ 1 - \Delta \kappa\) STEP \ \Delta \kappa} (integration)
\end{enumerate}

\begin{align*}
l = 2 \text{Int}[(k + \eta)/2] + 1; \ \bar{\kappa} = p - m & \quad (\text{cf. Eq. (B.1)}) \\
l' = 2 \text{Int}[(k' + \eta)/2] + 1; \ \bar{\kappa}' = p' - l' & \\
S_{mm'} = S_{mm'} + \bar{w}(\eta) \rho_{\bar{\kappa}l'}(\bar{\kappa}', \bar{\kappa}')
\end{align*}

\text{NEXT } \eta

The algorithm for the second step of the two-step iteration (3.10), describing the Hamiltonian phase is very simple [see Eq. (3.15)]

\[\rho_{mm'}(\kappa, \kappa'; t + \Delta t) = \sum_{ll'} M_{mm'\ell'}(\kappa, \kappa') \tilde{\rho}_{ll'}(\kappa, \kappa')\]

The subroutines (B.2)—(B.4) constitute the backbone of the implementation of the two-step iteration (3.10).
B.1.2 CPU Time

The number of floating-point operations (FPO) for one iteration of the irreversible phase is \( I_D = (3 + N_\kappa)N_\rho \), while for one iteration of the Hamiltonian phase \( I_H = 4N_m^2N_\rho \), which makes a total of \( I \equiv I_H + I_D = (3 + N_\kappa + 4N_m^2)N_\rho \) FPO per time-step (the array elements are complex).

The number of branches taken into account for the diagonalization of the Hamiltonian at the beginning of each run, \( N_B \), was typically \( 20 \leq N_B \leq 150 \) leading in the worst case to a \( 150 \times 150 \) matrix to be diagonalized. The lower and upper cutoff value of \( m \) in the stationary Schrödinger equation (2.40) was chosen symmetrically around the \( m \)-values of the initial state (symmetric around zero for Bragg-resonances; symmetric around \( m_0 \) for the \((m_0,l)\)-Doppleron-resonances with \( m_0 \gg l \geq 1 \)).

For the iteration, much computer time was saved by restricting the range of \( m \)-values of the \( \rho \)- and \( M \)-matrix to those, for which the states \(|\kappa,m\rangle \) get populated during the interaction time. This resulted in typical numbers of branches \( N_m = 6 \ldots 50 \).

The number of partitions of the Brillouin zone, \( N_\kappa \equiv 2/\Delta \kappa \), is determined by the momentum-resolution \( \Delta \kappa \). We found \( \Delta \kappa = 1/4 \) satisfactorily, i.e. \( N_\kappa = 8 \). In combination with the typical number of branches, \( N_m \), this led to a typical number of (complex) array-elements \( N_\rho \equiv (N_mN_\kappa)^2 = 2,304 \ldots 160,000 \) to be stored and propagated. From this, and the formula given at the beginning of this subsection, we obtain the typical number of floating-point operations \( I \approx 0.6 \text{MFLOPS} \ldots 3 \text{GFLOPS} \), which implies a typical CPU time of \( \approx 0.1 \ldots 500 \text{sec per unit step} \) on an IBM 6000 RISC workstation.
APPENDIX B. NUMERICAL IMPLEMENTATION

The time-scale $\Delta t$ was chosen to resolve the highest appearing system frequency given by the largest energy-difference of the populated eigenstates (energy bands) of $H$. For the maximum interaction-times considered, we found 100-200 time steps to provide for sufficient resolution. To give some examples, the overall CPU time used for figure (7) was 4h and for figure (11) it was 30min.

B.1.3 Remarks

The above algorithm is easily modified to take into account a non-trivial laser profile. This merely requires the subsequent diagonalization of $H$ and re-evaluation of $U$ and $M$. We found about 12 re-evaluations sufficient for a Gaussian profile realized under experimental conditions.

In all cases where spontaneous emission may be neglected, it is advisable to propagate the Schrödinger state-vector with $U$ instead of propagating $\rho$ with $M$. This reduces the one-step complexity from $N_\kappa^2 N_m^4$ to $N_\kappa N_m^2$. In this scheme, the evolution of non-pure states are easily simulated by averaging the results of the coherent evolution over an appropriate distribution of pure initial states. Similarly, an averaging of the results of the coherent evolution over a range of interaction times may be used to simulate the velocity spread of the incoming atoms.
In this appendix we derive the resonance conditions for both the Bragg and Doppleron resonances. Throughout the appendix we will use recoil units, i.e. frequencies are scaled with $\omega_{\text{rec}}$ and energies with $E_{\text{rec}}$.

**C.1 Bragg Resonances**

For the discussion of Bragg resonances it is convenient to introduce separate wave functions $e(x, t)$ and $g(x, t)$ for the upper and lower electronic state of the atom, respectively. In the coordinate representation the Schrödinger equation in recoil units then reads

\[
\begin{align*}
\frac{i}{\hbar} \dot{e}(x, t) &= -\frac{\partial^2}{\partial x^2} e(x, t) - \delta e(x, t) + R \cos(x) g(x, t) \\
\frac{i}{\hbar} \dot{g}(x, t) &= -\frac{\partial^2}{\partial x^2} g(x, t) + R \cos(x) e(x, t)
\end{align*}
\]

(C.1)

In the case of $\delta \gg R$ we can adiabatically eliminate the upper level if we assume the atom to be initially in the lower state. We can solve the first equation of (C.1) approximately
resulting in
\[ e(x, t) \approx \frac{\mathcal{R}}{\delta} \cos(x) g(x, t) \] (C.2)

which we can insert in the second equation to yield
\[ i\dot{g}(x, t) = -\frac{\partial^2}{\partial x^2} g(x, t) + \frac{\mathcal{R}^2}{\delta} \cos^2(x) g(x, t). \] (C.3)

The same approach can be taken to eliminate the lower level if the atom is initially in the upper state.

We now expand the wave function \( g(x, t) \) in Fourier components
\[ g(x, t) = \sum_m g_m(t) e^{ix}. \] (C.4)

with time dependent coefficients \( g_m(t) \). Here we have already taken into account the geometrical fact that the Bragg resonances are located in the middle and at the edges of the Brillouin zone, implying that only those momentum states are populated for which \( p = m\hbar q \). We proceed by transforming equation (C.3) to the \( p \)-representation, recognizing that the \( \cos^2(qx) \) term on the right hand side translates into a shift operator with
\[ \cos^2(x)|p\rangle = \frac{1}{2} \left( |p\rangle + \frac{1}{2}|p + 2\rangle + \frac{1}{2}|p - 2\rangle \right). \] (C.5)

After projection on the momentum eigenstate \( |m\rangle \) equation (C.4) and (C.3) yield then the
infinite set of equations

\[ ig_m(t) = n^2 g_m(t) + 2\epsilon g_m(t) + \epsilon(g_{m+2}(t) + g_{m-2}(t)) \]  \hspace{1cm} (C.6)

where we have introduced the dimensionless parameter \( \epsilon \)

\[ \epsilon = \frac{R^2}{4\delta} \]  \hspace{1cm} (C.7)

We now consider the specific Bragg resonance between \( p = \pm l \). In order to eliminate the nonresonant levels from the infinite set of equations (C.6) we first make the variable transformation

\[ g_m(t) = \tilde{g}_m(t)e^{-i(l^2+2\epsilon)t} \]  \hspace{1cm} (C.8)

resulting in equations

\[ \dot{\tilde{g}}_{\pm l}(t) = \epsilon(\tilde{g}_{\pm l+2}(t) + \tilde{g}_{\pm l-2}(t)) \]  \hspace{1cm} (C.9)

for the resonance levels \( \tilde{g}_{\pm l} \), and

\[ \dot{\tilde{g}}_m = (m^2 - l^2)\tilde{g}_m + \epsilon(\tilde{g}_{m+2} + \tilde{g}_{m-2}) \]  \hspace{1cm} (C.10)

for all other levels \( \tilde{g}_m \). We now eliminate the levels between the resonant levels in order to find the frequency of oscillation between the two resonant levels (corresponding to the energy gap \( \Delta E \) in the band scheme).
Because of the term \((m^2 - l^2) \gg 1\) on the right side of the equations for the nonresonant levels we can approximately set

\[
\dot{g}_m \approx 0
\]  
(C.11)

for \(m \neq \pm l\). We can then write equation (C.10) for the intermediate levels as

\[
\begin{pmatrix}
D_{-l+2} & \epsilon & 0 & \ldots & 0 \\
\epsilon & D_{-l+4} & \epsilon & \ldots & 0 \\
0 & \ldots & \epsilon & D_{l-4} & \epsilon \\
\vdots & \vdots & \epsilon & D_{l-4} & \epsilon \\
0 & \ldots & 0 & \epsilon & D_{l-2}
\end{pmatrix}
\begin{pmatrix}
\tilde{g}_{-l+2} \\
\tilde{g}_{-l+4} \\
\vdots \\
\tilde{g}_{l-4} \\
\tilde{g}_{l-2}
\end{pmatrix} =
\begin{pmatrix}
\tilde{g}_{-l} \\
0 \\
\vdots \\
0 \\
\tilde{g}_l
\end{pmatrix}
\]  
(C.12)

where the diagonal elements are given by \(D_d = d^2 - l^2\), and use Cramers rule to solve \(g_{-l+2}\) approximately as a function of \(g_l\) which, when inserted into the equation for \(g_{-l}\), allows the determination of the oscillation frequency we are looking for. From Cramers rule

\[
g_{-l+2} = \frac{\det A}{\det A'}
\]  
(C.13)

where \(A\) is the matrix on the left side of (C.12), and \(A'\) is the same matrix with the first column replaced by the vector on the right hand side of the equation. For \(\epsilon \ll 1\) the determinant of \(A\) can approximately be calculated as the product of the diagonal elements. And instead of calculating the total determinate of \(A'\) we calculate only the term proportional
APPENDIX C. RESONANCE CONDITIONS

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to \( b_l \) which is straightforward to do. As result we find

\[
g_{l+2} \approx \frac{\epsilon^{(l-1)}}{4(l-1)[(l-1)]^2} g_l + \alpha g_{-l}
\]

where \( \alpha \) needs not be determined any further. Taking into account the factor \( \epsilon \) in front of \( g_{l+2} \) in equation (C.9) we can finally write down the energy gap for the \( l \)-th order Bragg resonance as

\[
\Delta E_{\text{Bragg}} \approx \frac{\epsilon^l}{4(l-1)[(l-1)]^2}.
\]

C.2 Dopplerons

We now review the \( l \)-th order Doppleron resonance in which a ground state atom with transverse momentum \( m_0 \) is resonantly scattered into a state where the atom is excited, and moves with transverse momentum \( m_1 = m_0 + 2l + 1 \). To zeroth order in the atom-laser coupling, this process is resonant for a detuning \( \delta^{(0)} = m_1^2 - m_0^2 \) which compensates the difference in the kinetic energy gained by the scattered atom. As mentioned in the text, this resonance condition is expected to be modified due to AC Stark shifts induced by the nonresonant electro-translational levels when the laser interaction is taken into account.

To explain the dynamics of a particular Doppleron resonance, and to derive the precise resonance condition, we solve the Schrödinger equation

\[
\dot{c}_m(t) = E_m^{(0)} c_m(t) - \frac{\mathcal{R}}{2} (c_{m+1}(t) + c_{m-1}(t)), \quad m = 0, \pm 1, \pm 2, \ldots
\]
subject to the initial condition \( c_m(0) = \delta_{m,m_0} \). The incoming atom is assumed to be in the
electronic ground state, \( m_0 \) is assumed to be even, and \( \kappa = 0 \). Under these conditions

\[
E_m^{(0)} = m^2 - \frac{1 - (-1)^m}{2}\delta.
\]  
(C.17)

To allow for a \( l \)th order Doppleron resonance, we assume \( \delta \approx \delta^{(0)} \equiv m_1^2 - m_0^2 \), such that

\[
E_m^{(0)} \approx E_m^{(0)} \quad \text{where} \quad m_1 \text{ stands for } m_0 + 2l + 1.
\]

Observing the symmetry \( E_m^{(0)} = E_{-m}^{(0)} \), the set (C.16) is transformed into two decoupled sets for the amplitudes \( s_m = c_m + c_{-m} \) and \( d_m = c_m - c_{-m} \), collectively referred to as \( Q_m \).

The modified Laplace transform

\[
\tilde{Q}(z) = -i \int_0^\infty e^{izt}Q(t)dt
\]

then yields algebraic equations of the form

\[
D_m(z)\tilde{Q}_m(z) + \frac{\mathcal{R}}{2}\tilde{Q}_2(z) = 0,
\]

\[
D_m(z)\tilde{Q}_m(z) + \frac{\mathcal{R}}{2}(\tilde{Q}_{m-1}(z) + \tilde{Q}_{m+1}(z)) = \delta_{m,m_0}, \quad m = 2, 3, \ldots,
\]  
(C.18)

where \( D_m(z) = z - E_m^{(0)} \) for \( m \geq 2 \). For \( m = 1 \) and \( Q=s \) we have \( D_1(z) = z - E_1^{(0)} - \mathcal{R}^2/2(z - E_0^{(0)}) \), while \( D_1(z) = z - E_1^{(0)} \) if \( Q=d \).

A perturbative solution of the set of equations (C.18) is threatened by a secular divergence resulting from the Doppleron degeneracy \( E_{m_0}^{(0)} \approx E_{m_1}^{(0)} \) which calls for a separate treatment of those two equations where \( m = m_0 \) and \( m = m_1 \). Using standard techniques
to formally eliminate from Eqs. (C.18) all but the pair of potentially resonant amplitudes
Q_{m_0} and Q_{m_1}, the equations for the latter take the form

\[
\begin{pmatrix}
A(z) & G(z)
\end{pmatrix}
\begin{pmatrix}
\tilde{Q}_{m_0}(z)
\tilde{Q}_{m_1}(z)
\end{pmatrix} =
\begin{pmatrix}
1 \\
0
\end{pmatrix},
\]

(C.19)

where

\[
A(z) = z - E^{(0)}_{m_0} - \frac{\mathcal{R}^2}{4} \left( T^+_{m_0,m_0-1}(z) + T^-_{m_0+1,m_0-1}(z) \right),
\]

(C.20)

\[
B(z) = z - E^{(0)}_{m_1} - \frac{\mathcal{R}^2}{4} \left( T^-_{m_1+1,m_0}(z) + T^+_{m_0+1,m_1-1}(z) \right),
\]

(C.21)

\[
G(z) = \frac{(\mathcal{R}/2)^{2l+1}}{\Delta_{m_0+1,m_1-1}(z)}.
\]

(C.22)

Here \( \Delta_{m,n} \) denotes the determinant of a tridiagonal \((n - m + 1) \times (n - m + 1)\) square matrix with diagonal elements \(D_m, D_{m+1}, \ldots, D_n\) and \(\mathcal{R}/2\) off diagonal. In terms of those determinants, the auxiliary quantities \(T^\pm_{m,n}\) are given by \(T^+_{m,n} = \Delta_{m,n-1}/\Delta_{m,n}\), \(T^-_{m,n} = \Delta_{m+1,n}/\Delta_{m,n}\), and have the continued fraction representation

\[
T^+_{m,n}(z) = \frac{1}{D_n(z) - (\mathcal{R}/2)^2 T^+_{m,n-1}(z)},
\]

(C.23)

\[
T^-_{m,n}(z) = \frac{1}{D_m(z) - (\mathcal{R}/2)^2 T^-_{m+1,n}(z)}.
\]

(C.24)

Equations (C.19) are easily solved with the result \(\tilde{Q}_{m_0}(z) = B(z)/D(z)\), \(\tilde{Q}_{m_1}(z) = -G(z)/D(z)\), where \(D(z) \equiv A(z)B(z) - G(z)^2\) is the determinant of the 2 \(\times 2\) matrix in Eq. (C.19). The zeros of this determinant are all real. They give the position of the poles.
in the inverse Laplace transform $Q(t) = \int e^{-ist} \tilde{Q}(z) dz/2\pi i$ which, being evaluated as a contour integral, renders $Q(t)$ as a sum of oscillating exponentials with frequencies given by the zeros of $\mathcal{D}(z)$ and amplitudes given by the residues of $Q(z)$ at the corresponding poles.\footnote{The poles of $B(z)$ and $G(z)$ do not contribute since they are canceled by the same poles in $\mathcal{D}(z)$.}

As it stands, the problem of finding the zeros of $\mathcal{D}(z)$ and corresponding residues is a perfect candidate for a numerical solution, the only "complicated" routine required being a root finding algorithm à la Newton-Raphson. In fact, due to the distinctive treatment of the potentially resonant amplitudes $Q_{m_0}$ and $Q_{m_1}$, the determinant $\mathcal{D}(z)$ is exceptionally well behaved near the two roots $z_1$ and $z_2$ which approach the unperturbed frequencies $E^{(0)}_{m_0}$ and $E^{(0)}_{m_1}$ of $Q_{m_0}$ and $Q_{m_1}$ in the limit $\mathcal{R} \rightarrow 0$. In particular, the distinctive treatment of $Q_{m_0}$ and $Q_{m_1}$ has removed all spurious singularities, which generally plague continued fractions.

Concentrating for the time being on the two zeros $z_1, z_2$ of $\mathcal{D}(z)$ associated with $Q_{m_0}$ and $Q_{m_1}$, we write $\mathcal{D}(z) = (z - z_1)(z - z_2)F(z)$. Here the function $F(z)$ is expected—and subsequently demonstrated—to be a well behaved function of order one, with zeros only "far off" the resonance frequencies $z_{1,2}$.

Denoting $\Delta E = z_1 - z_2$, $E_c = (z_1 + z_2)/2$, and applying the inverse Laplace transform, our favorite amplitudes turn out to evolve in time according to

$$
\begin{pmatrix}
Q_{m_0}(t) \\
Q_{m_1}(t)
\end{pmatrix}
= \frac{e^{-iE_c t}}{\Delta E}
\begin{pmatrix}
B_1 e^{-i\Delta E t/2}/F_1 - B_2 e^{i\Delta E t/2}/F_2 \\
-G_1 e^{-i\Delta E t/2}/F_1 + G_2 e^{i\Delta E t/2}/F_2
\end{pmatrix}
+ \begin{pmatrix}
R_{m_0}(t) \\
R_{m_1}(t)
\end{pmatrix}
$$

(C.25)

where $B_1 = B(z_1)$ etc., and the $R_m(t)$ denote contributions from the inverse Laplace trans-
form associated with the (far remote) zeros of $F(z)$. Below we shall show that these contributions are comparably small in a resonant situation.

From Eq. (C.25) we may read off that $Q_{m_0}(t)$ and $Q_{m_1}(t)$ are "in resonance"—i.e oscillate with equal amplitudes—if we can adjust the two roots $z_1, z_2$ by a proper choice of the experimental parameters (the detuning) such that $|G(z_{1,2})| = |B(z_{1,2})|$. By virtue of the defining equation $A(z_{1,2})B(z_{1,2}) = G(z_{1,2})^2$, these requirements are in fact equivalent to the two conditions $A(z_{1,2}) = B(z_{1,2})$, called resonance conditions in what follows.

Having only the detuning to play with, the system of resonance conditions is overdetermined: the resonance conditions can never be fulfilled exactly. If not exactly, however, the resonance conditions can be fulfilled at least quite well if the atom-laser coupling is not too strong. This is of advantage anyway since a strong atom-laser interaction would lead to multiple beam splitting, which is not desired here.

In the remainder of this appendix we leave the exact description behind and turn to perturbation theory in order to investigate the Doppleron resonances further. Any reader who has little time is advised to skip the following paragraphs, and to jump directly to the final statements around Eqs. (C.37)–(C.39).

Introducing the small parameter

$$\epsilon = \max \left( \frac{\mathcal{R}/2}{E_{m_0}^{(0)} - E_{m_1}^{(0)}}, \frac{\mathcal{R}/2}{E_{m_0}^{(0)} - E_{m_1}^{(0)}} \right) \approx \frac{\mathcal{R}}{8m_0}, \quad (C.26)$$

we observe $G(z)$ [see Eq. (C.22)] to be of order $\mathcal{R}e^{2It}$ in the relevant range of $z$. Since in this
range the derivative \( dG(z)/dz \) is of order \( 2\epsilon^{2l+1} \ll 1 \), we may replace the function \( G(z) \), and in particular the residue parts \( G(z_{1,2}) \) by the effective coupling constant

\[
G = (\mathcal{R}/2)^{m_0-1} \prod_{m=m_0+1}^{m_1} \frac{(\mathcal{R}/2)}{E_m^{(0)} - E_m^{(0)}} = (-1)^{l} \frac{\mathcal{R}}{2} \frac{(\mathcal{R}/8)^{2l}m_0!}{(l!)^2(m_0 + 2l)!}, \tag{C.27}
\]

neglecting corrections of order \( \epsilon^{2l+1} \). For later usage we also note that

\[
\frac{d}{dz} A(z) \sim \frac{d}{dz} B(z) \sim 1 + O(\epsilon^2), \tag{C.28}
\]

\[
\frac{d^2}{dz^2} A(z) \sim \frac{d^2}{dz^2} B(z) \sim \frac{1}{m_0} O(\epsilon^2), \tag{C.29}
\]

which is easily proved by inserting the leading order \( T^{+}_{1,m_0-1}(z) \approx 1/(z - E_{m_0-1}^{(0)}) \) etc. into the defining equations (C.20) and (C.21) of \( A(z) \) and \( B(z) \), respectively, and taking the \( z \)-derivatives.

To find the zeros \( z_1 \) and \( z_2 \) of \( D(z) \), we use the parametrization \( z_{1,2} = E_c \pm \Delta E/2 \), and expand \( A(z) \) and \( B(z) \) around the (yet unknown) center \( E_c \). Writing short \( A_c \) for \( A(E_c) \) etc., and using Eqs. (C.27)–(C.29), the leading order of the defining equations \( D(z_{1,2}) = 0 \) reads

\[
A_c B_c \pm (A_c + B_c) \Delta E/2 + (\Delta E/2)^2 = G^2 \text{ which imposes the condition}
\]

\[
A(E_c) + B(E_c) = 0, \tag{C.30}
\]

and implies the solution

\[
\Delta E = 2\sqrt{G^2 + A_c^2}. \tag{C.31}
\]
The values $B(z_{1,2})$ and $F(z_{1,2})$ which in combination with $\Delta E$ determine the amplitudes of $Q_{m_0}(t)$ and $Q_{m_1}(t)$, respectively, are obtained similarly. To determine the regular part $F(z)$ in $A(z)B(z) - G(z)^2 = (z - z_1)(z - z_2)F(z)$, we expand $A(z)$ and $B(z)$ around $E_c$, observe Eqs. (C.27)-(C.31) to obtain

\[
B(z_{1,2}) = -A(E_e) \pm \Delta E/2, \tag{C.32}
\]

\[
F(z_{1,2}) = 1, \tag{C.33}
\]

up to relative corrections of order $\epsilon^2$. Now everything depends on the (yet unknown) center frequency $E_c$ and the value $A_e = A(E_c)$.

To proceed, we impose the resonance condition $A(z_{1,2}) = B(z_{1,2})$ which reads $A(E_e) = B(E_e)$ up to corrections of order $\Delta E \epsilon^2$. In combination with the center condition (C.30) we then have to solve $A(E_e) = 0$, i.e.

\[
E_e = E^{(0)}_{m_0} + \frac{\mathcal{R}^2}{4} \left( T^+_{1,m_0-1}(E_e) + T^-_{m_0+1,m_1-1}(E_e) \right). \tag{C.34}
\]

The solution $E_e = E_e(\delta)$ of this equation still has to obey the resonance condition $A(E_e(\delta)) = B(E_e(\delta))$, i.e. [see Eqs. (C.20),(C.21)]

\[
\delta = m_1^2 - m_0^2 - \frac{\mathcal{R}^2}{4} \left( T^+_{1,m_0-1}(E_e) + T^-_{m_0+1,m_1-1}(E_e) \right) \tag{C.35}
\]

\[
+ \frac{\mathcal{R}^2}{4} \left( T^-_{m_1+1,\infty}(E_e) + T^+_{m_0+1,m_1-1}(E_e) \right), \tag{C.36}
\]
which in turn fixes the optimal detuning $\delta_r = \delta(R)$ and yields the center frequency $E_{cr} = E_c(\delta_r)$ up to relative corrections of order $\epsilon^{2l+2}$. Below we will outline an iterative procedure to solve Eqs. (C.34) and (C.36) simultaneously. We assume for now to have found their solutions $\delta_r$ and $E_{cr}$ and study the impact of small deviations $\Delta \delta = \delta - \delta_r$ on the resonance performance of our favorite amplitudes. These deviations lead to a modification of the center frequency $\Delta E_c = E_c - E_{cr}$ which is determined by the center condition $A(E_{cr} + \Delta E_c, \delta_r + \Delta \delta) + B(E_{cr} + \Delta E_c, \delta_r + \Delta \delta) = 0$. To first order in the deviations and to leading order in $\epsilon$, the solution of this equation is $\Delta E_c = -\Delta \delta/2$, which leads to $A_c = -\Delta \delta/2$. Including deviations $\Delta k$ of the momentum of the impinging atom, similar reasoning leads to $\Delta E_c = (m_0 + m_1)\Delta k - \Delta \delta/2$ and

$$A_c = (2l + 1)\Delta k - \frac{\Delta \delta}{2}, \quad (C.37)$$

which completes the perturbative analysis of our resonance. Using Eq. (C.37) in Eqs. (C.31)–(C.33), inserting the resultant expressions in Eq. (C.25), and using the definition of $Q_m(t)$ in terms of sums and differences of $c_m(t)$, the result is

$$c_{ma}(t) = e^{-iEt} \left( \cos(\Delta Et/2) + i \frac{A_c}{\sqrt{G^2 + A_c^2}} \sin(\Delta Et/2) \right) + R_{ma}(t), \quad (C.38)$$

$$c_{m1}(t) = i \frac{G}{\sqrt{G^2 + A_c^2}} e^{-iEt} \sin(\Delta Et/2) + R_{m1}(t), \quad (C.39)$$

where the remainders $R_m(t)$ are of order $\epsilon$ and $A_c$ is given in Eq. (C.37). The probability
to find the atom moving with momentum \( m_1 + \Delta k \)

\[
|c_{m_1}(t)|^2 = \frac{1}{1 + \frac{A^2_c}{G^2}} \frac{1}{2} \left[ 1 - \cos \left( \sqrt{G^2 + A^2_c t} \right) \right]
\] (C.40)

reveals oscillations with an amplitude which has the form of a two dimensional Lorentzian. The respective widths are given by

\[
\Delta \delta^{HWHM} = 2G = \mathcal{R} \frac{\mathcal{R}^{2l} m_0!}{6^l (4!)^2 (m_0 + 2l)!},
\] (C.41)

and

\[
\Delta k^{HWHM} = \frac{G}{2l + 1} = \frac{\Delta \delta^{HWHM}}{4l + 2},
\] (C.42)

meaning that the momentum transfer of the Doppleron decreases to less than half the optimal value when detuning or the initial momentum deviate more than the above widths from their respective resonance values \( \delta_r \) and \( m_0 \).

This reminds us that we still need to solve Eqs. (C.36) and (C.34) for the optimal detuning \( \delta_r \) and corresponding center frequency \( E_{cr} \). These equations have the structure \( E_c = \mathcal{F}(E_c, \delta) \), \( \delta = \mathcal{G}(E_c, \delta) \) and are most easily solved using an iteration scheme. Introducing the notation \( E^{(j)}_c \) and \( \delta^{(j)} \) for the \( j^{th} \) approximant, we set up the iteration \( E^{(j+1)}_c = \mathcal{F}(E^{(j)}_c, \delta^{(j)}) \) and similarly \( \delta^{(j+1)} = \mathcal{G}(E^{(j)}_c, \delta^{(j)}) \) with the initial values \( E^{(0)}_c = E^{(0)}_{m_0} \) and \( \delta^{(0)} = m_1^2 - m_0^2 \). To be consistent in calculating the \( j^{th} \) approximant, the continued fractions in Eqs. (C.34) and (C.36) have to be truncated at the \( j^{th} \) level, and the \( (j - m)^{th} \)
approximants should be used on the \( m^{th} \) intermediate level. Following all these recipes, we have to iterate up to \( j = l \) and may identify \( E_{cr} = E_c^{(l)} \) and \( \delta_r = \delta^{(l)} \), respectively.

The first approximants are readily obtained

\[
E_c^{(1)} = m_0^2 + (\mathcal{R}/4)^2 \left[ \frac{1}{(m_0 + l)(l + 1)} + \frac{1}{(m_0 + l + 1)(l + 1)} \right], \tag{C.43}
\]
\[
\delta^{(1)} = \delta^{(0)} - \mathcal{R}^2 \frac{2l + 1}{16l(l + 1)} \left[ \frac{1}{m_0 + l + 1} + \frac{1}{m_0 + l} \right], \tag{C.44}
\]

but the general expressions for the second approximants are already very messy and opaque.

To give an impression, we give the second (and final) approximant of a second order Doppler resonance \( (l = 2) \) \[50\]

\[
\delta_r \equiv \delta^{(2)} = \delta^{(0)} + \frac{5\mathcal{R}^2}{96} \left[ \frac{N_1 + N_2}{m_0 + 2} + \frac{N_3 + N_4}{m_0 + 3} \right], \tag{C.45}
\]

where

\[
N_1 = \frac{3}{5} \left[ 1 - \frac{\mathcal{R}^2}{128(m_0 + 2)} \left( \frac{1}{3(m_0 + 2)} + \frac{1}{2(m_0 + 3)} - \frac{1}{m_0 + 4} \right) \right]^{-1}, \tag{C.46}
\]
\[
N_2 = \frac{2}{5} \left[ 1 - \frac{\mathcal{R}^2}{192(m_0 + 2)} \left( \frac{1}{m_0 - 1} + \frac{1}{2(m_0 + 2)} + \frac{1}{3(m_0 + 3)} \right) \right]^{-1}, \tag{C.47}
\]
\[
N_3 = \frac{3}{5} \left[ 1 - \frac{\mathcal{R}^2}{128(m_0 + 3)} \left( \frac{1}{3(m_0 + 3)} + \frac{1}{2(m_0 + 2)} - \frac{1}{m_0 + 1} \right) \right]^{-1}, \tag{C.48}
\]
\[
N_4 = \frac{2}{5} \left[ 1 - \frac{\mathcal{R}^2}{192(m_0 + 3)} \left( \frac{1}{m_0 + 6} + \frac{1}{2(m_0 + 3)} + \frac{1}{3(m_0 + 2)} \right) \right]^{-1}. \tag{C.49}
\]
In particular, for the second order Doppleron with $m_0 = 600$ and $R = 4000$ we find [50]

$$\delta_r = \delta^{(0)} + (\delta^{(1)} - \delta^{(0)}) + (\delta^{(2)} - \delta^{(1)}) = 6625 - 2516 - 512 = 3597.$$  \hspace{1cm} (C.50)

We also have $\Delta \delta^{HWHM} = 324$, i.e. the second correction exceeds the bandwidth and neglecting it will certainly suppress the desired resonance.
LIST OF REFERENCES


LIST OF REFERENCES


[51] This number was chosen with the prospect of an experiment suggested in the Ph.D. thesis of B. Oldaker (1990).


