Optimal atomic detection by control of detuning and spatial dependence of laser intensity

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Abstract. Atomic detection by fluorescence may fail because of reflection from the laser or transmission without excitation. The detection probability for a given velocity range may be improved by controlling the detuning and the spatial dependence of the laser intensity. A simple optimization method is discussed and exemplified.

PACS numbers: 03.65.-w, 42.50-p, 32.80-t
1. Introduction

One of the standard ways to measure the time of flight, or simply the presence of an atom, consists of illuminating it with a laser and detect the induced fluorescence. There are many different experimental settings depending on the incident atomic velocities and spatial span of the atomic cloud or beam. In particular, the light of the probe laser may be spread as a broad sheet perpendicular to the atomic motion or be focused onto a diameter of a few microns; it may also be continuous or pulsed. These detection schemes may fail however at low (ultracold) atomic velocities because of atomic reflection from a strong laser field; the atoms may also traverse the finite laser-illuminated region without emitting any photon even at moderate velocities if the laser intensity is weak.

Figure 1 illustrates these two phenomena. It represents the detection probability versus (ultracold) atomic velocity for a given laser-beam width \( L = 10 \mu \text{m} \). (This and other figures are obtained for the transition at 852 nm of Cs atoms, with \( \gamma = 33.3 \times 10^6 \text{ s}^{-1} \).) \( \Omega = 0.1033 \times 10^6 \text{ s}^{-1} \) (solid line); \( \Omega = 5 \gamma \) (dashed line); in both cases \( \Delta = 0 \).

\[
\begin{array}{c|c c c c c c c c c c c}
\hline
v (\text{cm/s}) & 0 & 0.2 & 0.4 & 0.6 & 0.8 & 1 & 1.2 & 1.4 & 1.6 & 1.8 & 2 \\
A & 0 & 0.2 & 0.4 & 0.6 & 0.8 & 1 & 1.2 & 1.4 & 1.6 & 1.8 & 2 \\
\hline
\end{array}
\]

**Figure 1.** Detection probability versus velocity \( v \) for laser beam width \( L = 10 \mu \text{m} \). (This and other figures are obtained for the transition at 852 nm of Cs atoms, with \( \gamma = 33.3 \times 10^6 \text{ s}^{-1} \).) \( \Omega = 0.1033 \times 10^6 \text{ s}^{-1} \) (solid line); \( \Omega = 5 \gamma \) (dashed line); in both cases \( \Delta = 0 \).
The objective of this paper is to show that an appropriate adjustment of detuning and of the position dependence of the laser intensity may indeed achieve this goal.

In the next section we shall present the theory to model the atom detection, section III describes the optimization of laser intensity and detuning, and in section IV we provide a numerical example.

2. Basic theory

The fundamental theory for the modeled experiment is described in Refs. [1], [2] and [3]. A two-level atom with transition frequency $\omega$ impinges along the $x$ direction on a perpendicular continuous laser beam of frequency $\omega_L$ directed along the $y$ direction. In the so called quantum jump approach [4] the continuous measurement of the fluorescence photons is simulated by a periodic projection onto no-photon or one-photon subspaces every $\Delta t$, a time interval large enough to avoid the Zeno effect, but smaller than any other characteristic time. The amplitude for the wavepacket of undetected atoms in the interaction picture for the internal Hamiltonian obeys, in a time scale coarser than $\Delta t$, and using the rotating wave and dipole approximations, an effective Schrödinger equation governed by the complex “conditional” Hamiltonian (the hat is used to distinguish momentum and position operators from the corresponding c-numbers)

$$H_{c,3D} = \frac{\hat{p}^2}{2m} + \frac{\hbar}{2} \Omega(\hat{x}) \left\{ |2\rangle\langle 1|e^{ikL\hat{y}} + \text{h.c.} \right\}$$

$$- \frac{\hbar}{2} (2\Delta + i\gamma)|2\rangle\langle 2|,$$

(1)

where $\gamma$ is the Einstein coefficient of the excited level (level 2), i.e. its decay rate or inverse life time, $\Omega(x)$ is the position dependent Rabi frequency (assumed to be real), $\Delta = \omega_L - \omega$ is the detuning, and $\hat{p}$ is the momentum operator in three dimensions (3D). The factor $e^{ikL\hat{y}}$ takes into account the spatial dependence of the laser coupling. A one dimensional model is obtained by assuming that the atomic wave packet is centered at $y = 0$ and satisfies $k_L \Delta y \ll 1$ before the first photon emission, so that the exponentials can be dropped and a one dimensional kinetic term suffices [2],

$$H_c = \frac{\hat{p}^2}{2m} + \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega(\hat{x}) \\ \Omega(\hat{x}) & -i\gamma - 2\Delta \end{pmatrix},$$

(2)

where $\hat{p}$ is the momentum operator conjugate to $\hat{x}$, the ground state $|1\rangle$ is in vector-component notation $|1\rangle_0$, and the excited state $|2\rangle$ is $|0\rangle_1$. The probability, $N_t$, of no photon detection from $t_0$, the instant when the packet is prepared far from the laser and with positive momenta, up to time $t$, is given by [4]

$$N_t = |\langle e^{-iH_c(t-t_0)/\hbar}|\psi(t_0)\rangle|^2,$$

(3)

where $|\psi(t_0)\rangle$ is the (two-component) wave vector at $t_0$, and the probability density, $\Pi(t)$, for the first photon detection by

$$\Pi(t) = -\frac{dN_t}{dt} = \gamma P_2,$$

(4)
where \( P_2 \) is the population of the excited state.

To obtain the time development under \( H_c \) of a wave packet incident from the left we solve first the stationary equation

\[
H_c \Phi = E \Phi, \quad \text{where } \Phi(x) \equiv \begin{pmatrix} \phi^{(1)}(x) \\ \phi^{(2)}(x) \end{pmatrix}
\]

for scattering states with real energy \( E = \hbar^2 k^2 / 2m = E_k \), which are incident from the left \( (k > 0) \),

\[
\Phi_k(x) = \frac{1}{\sqrt{2\pi}} \left\{ \begin{array}{l}
\left(e^{ikx} + R_1 e^{-ikx}\right), \quad x \sim -\infty, \\
\left(T_1 e^{ikx} - T_2 e^{-iqx}\right), \quad x \sim \infty.
\end{array} \right.
\]

These states are not orthogonal, in spite of the reality of \( E \), because the Hamiltonian \( H_c \) is not Hermitian. The wavenumber \( q \) obeys

\[
E + i\hbar \gamma / 2 = \hbar^2 q^2 / 2m,
\]

with \( \text{Im} \quad q > 0 \) for boundedness, while \( R_{1,2} \) and \( T_{1,2} \) are reflection and transmission amplitudes for the ground and excited state channels.

If \( \tilde{\psi}(k) \) denotes the wavenumber amplitude that the wave packet would have as a freely moving packet at \( t = 0 \), then

\[
\Psi(x, t) = \int_0^\infty dk \, \tilde{\psi}(k) \Phi_k(x) e^{-i\hbar k^2 t / 2m}
\]
describes the “conditional” time development of the state for an undetected atom which in the remote past comes in from the left in the ground state.

Some simple forms of \( \Omega(x) \) admit analytical solutions for the stationary waves, as demonstrated in [1, 3], but we shall limit the present discussion to an approximation that is valid for “arbitrary” shapes of \( \Omega \) within weak driving and low energy conditions [5].

Equation (5) reads explicitly

\[
- \frac{\hbar^2}{2m} \frac{\partial^2 \Phi^{(1)}(x)}{\partial x^2} + \frac{\hbar}{2} \Omega(x) \Phi^{(2)}(x) = E \Phi^{(1)}(x),
\]

\[
- \frac{\hbar^2}{2m} \frac{\partial^2 \Phi^{(2)}(x)}{\partial x^2} + \frac{\hbar}{2} \Omega(x) \Phi^{(1)}(x) - \frac{\hbar}{2} (2\Delta + i\gamma) \Phi^{(2)}(x) = E \Phi^{(2)}(x).
\]

In the large \( \gamma \) limit,

\[
\frac{\hbar |2\Delta + i\gamma|}{2} \gg \frac{\hbar}{2} \Omega, E,
\]

we may neglect the kinetic and energy terms in the second equation to write

\[
\Phi^{(2)} = \frac{\Omega}{2\Delta + i\gamma} \Phi^{(1)}.
\]

Physically, it is assumed that the excited state amplitude is small and proportional to the ground state amplitude, because the depletion by decay is rapid with respect to the
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atomic motion and to the Rabi pumping period. Substituting (12) into (9), there results a closed, one channel equation for $\Phi^{(1)}$ with a complex potential

$$V(x) = \frac{\hbar \Omega^2(x)}{2} \frac{\Delta + i\gamma}{\Delta^2 + \gamma^2},$$

so that the sign of the real part has the sign of the detuning whereas the imaginary part is negative, i.e. absorbing, for all $x$.

The complex potential for the longitudinal direction $x$ and a traveling laser wave perpendicular to the initial atomic motion is similar to the one that appears for the transversal direction $y$ using the Raman-Nath or related approximations to describe the incidence of the atom on perpendicular standing laser fields [5, 6]. In these approximations, however, $x$ is treated as a parameter according to $x = vt$ but $y$ is kept as a variable, whereas here $x$ is the variable and we consider the motion along a ray of constant $y = 0$.

Notice that, within the stated conditions, the potential is independent of $E$. This implies that all (low energy) stationary scattering functions are subject to the same potential and therefore the time dependent Schrödinger equation also reduces to an effective one channel equation with the effective potential $V$.

Within the one channel approximation, we have to find scattering solutions with the asymptotic form

$$\Phi^{(1)}(x) = \frac{1}{\sqrt{2\pi}} \begin{cases} e^{ikx} + R_1 e^{-ikx}, & x \sim -\infty, \\ T_1 e^{ikx}, & x \sim \infty. \end{cases}$$ (15)

The absorption (i.e. detection) probability $A(k)$ for the incident $k$-plane wave is given by

$$A(k) = 1 - |R_1|^2 - |T_1|^2.$$ (16)

3. Optimization

The main aim of the present paper is to show that the atomic detection may be improved by varying the spatial dependence of the laser intensity and the detuning. To get optimal dependences for a fixed total length of the laser illuminated region and for a given momentum range one has to find first, for weak driving conditions, the form of the complex potential that maximizes absorption.

A very similar objective (optimizing a complex absorbing potential) is also pursued in time-dependent molecular scattering calculations to eliminate the outgoing wave packets at the edge of the computational box and avoid unphysical effects [7, 10, 11, 12, 13]. We may take advantage of this coincidence by using, mutatis mutandis, similar optimization techniques. An obvious difference with the molecular scattering case is that here the real and imaginary parts of the potential have specific
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physical meanings in terms of laser parameters. In particular the detuning $\Delta$ and Rabi frequency $\Omega$ are given by

$$\Delta = -\frac{\gamma \text{Re}(V)}{2\text{Im}(V)};$$

$$\Omega = |V| \left(\frac{2\gamma}{-\hbar \text{Im}(V)}\right)^{1/2}.$$  

This means that not all absorbing potentials $V$ can be admitted, since the weak driving condition has to be satisfied, and moreover real and imaginary parts are not independent according to Eq. (17). The limitation of the weak driving condition may be avoided, but at the price of losing the simplified one-channel description, i.e., by keeping the two-channel equations and a $2 \times 2$ complex potential matrix. In the same manner one could also get rid of the limitation to small kinetic energies and optimize detection of thermal atoms, for example. Here we shall discuss the simple one-channel case.

The strategy is variational: we choose a functional form for $V$ that depends on a few parameters and then find the values of these parameters that maximize the absorption for a given velocity interval, or, in practice, for a discrete set of $n$ velocities in such an interval $[7],\quad \bar{A} \equiv \sum_j A(k_j)W(k_j).$  

The “weights” $W(k_j)$ may be chosen according to the momentum distribution of the atoms, or, as in the examples discussed below, uniformly for a chosen absorption window, $W(k_j) = 1/n$. In principle, it is possible to construct explicitly potentials that absorb perfectly at a discrete set of wavenumbers $[11]$, but these potentials tend to be too sensitive to small variations and thus ineffective for practical usage, and require in general arbitrary variations of real and imaginary parts. A further drawback in the present application is that they may have wild spatial variations or may correspond locally to strong driving conditions for which the one-channel, complex-potential model is not physically valid.

Moreover, an ideal potential functional form for optimizing atom detection should enable us to control the spatial scale in which the laser intensity varies significantly, in accordance with technical capabilities. A simple form would be the sum of contiguous Gaussian functions with a certain width. Independently of the optimization algorithm used many evaluations of $\bar{A}$ are required in general. Each of them requires to solve numerically the Schrödinger equation to obtain the amplitudes $T_1$ and $R_1$, and this may be very time consuming. Here we shall choose an even simpler functional form, a set of contiguous “square barriers”, as an approximation for a more realistic combination of Gaussians. At the present stage, where we are more interested in illustrating the concepts and general features involved than in any particular application, this simplification does not introduce any significant distortion $[3]$. The great numerical advantage of the square barriers is that the solution of the Schrödinger equation may be performed by multiplying a few $2 \times 2$ transfer matrices, which is an extremely
fast process in comparison to the numerical techniques required for other functional forms. Moreover one can write explicitly the gradient of $\bar{A}$ with respect to the real and imaginary parts of the barriers, so that very efficient optimization algorithms may be used. Expressions of the absorption and its gradient in terms of transfer matrices may be found in [11, 12, 13]. The main technical novelty here with respect to those works is the need to constrain the real and imaginary parts according to Eq. (17) and to weak driving conditions. Our subroutine for constrained optimization is based in the successive quadratic programming algorithm [14].

4. Results and discussion

Figure 2 shows the best absorption curves found for a range of momenta between 0.2 cm/s and 9 cm/s considering one and two barriers for a total length of 10 $\mu$m of the laser illuminated region, as in Figure 1. The potential, detuning and Rabi frequency corresponding to the optimal two-barrier case are shown in Figures 3 and 4. Note that the optimal single barrier fails at both edges of the momentum range chosen whereas two barriers, with three free parameters to optimize, do a much better job. We have also calculated an optimal eight barrier potential, see figures 5 and 6, that suggests that the form of an ideal continuous potential would be characterized by a smooth, non-linear increase of laser intensity with position, and negative detuning.

The present variational approach is based on a number of simplifying assumptions but the concepts involved are applicable even outside the domain of validity of these assumptions. In particular, the restriction to weak laser interactions and low energies is not fundamental and may be removed by considering the full $2 \times 2$ potential matrix instead of the one-channel effective potential. Similarly, more realistic and smooth functional forms may be used. We have assumed here that a number of laser beams with different intensity may be combined in a composite double (or multiple) beam to maximize the detection probability, but there are other simple possibilities to explore: Meneghini et al., for example, have considered a linear modulation of the detuning, that could be realized in a nonhomogeneous magnetic field, and a standard Gaussian form for the Rabi frequency [15]. This amounts to a four-parameter functional form for the potential, whose absorption may be also maximized for specific applications.

Apart from maximizing detection, there are other quantities that could be maximized or minimized, such as the detection delay. A minimal detection delay would be of interest for an accurate measurement of arrival times [1, 3, 16]. One possible application of a “perfect detector” in a broad momentum range, would be the measurement, for the first time, of the backflow effect, namely, negative current densities for an atomic wave packet composed by positive momenta [1, 16, 17, 18, 9]. This and other extensions of the present work will be dealt with elsewhere.
Figure 2. Absorption versus velocity $v$ for potentials optimized taking $n = 100$ between 0.2 and 9 cm/s in $[10]$. $L = 10 \, \mu m$. Solid line: two barriers (each of 5 $\mu m$); dashed line: one barrier; dots: eighth barriers.

Figure 3. Real (solid line) and imaginary part (dashed line) of the two-barrier potential of Figure 2.
Figure 4. Detuning (dashed line) and Rabi frequency (solid line) of the two-barrier potential of Figure 3.

Figure 5. Real (solid line) and imaginary part (dashed line) of an optimized eight-barrier potential. Other parameters as in figure 2.
Figure 6. Detuning (dashed line) and Rabi frequency (solid line) of the eight-barrier potential of figure 5.

Acknowledgments

We are grateful to J. P. Palao and S. Brouard for technical assistance. This work has been supported by Ministerio de Ciencia y Tecnología (BFM2000-0816-C03-03), UPV-EHU (00039.310-13507/2001), and a German-Spanish collaboration Grant.

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