RAPID COMMUNICATIONS

PHYSICAL REVIEW A VOLUME 44, NUMBER 5 1 SEPTEMBER 1991

Atomic deflection in the transition between diffractive and diffusive regimes: A numerical simulation

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(Received 11 April 1991)

The transition between diffractive and diffusive regimes in the deflection of atoms by a standing-wave light field has recently been observed experimentally by Gould *et al.* [Phys. Rev. A **43**, 585 (1991)]. We describe and present the results of a numerical simulation which allows these results to be understood in terms of the theory developed by Tanguy, Reynaud, and Cohen-Tannoudji [J. Phys. B **17**, 4623 (1984)].

I. INTRODUCTION

The study of the forces on atoms by light has been the subject of increasing theoretical and experimental research [1-3]. An experiment basic to our understanding of these forces has been realized by Gould *et al.* [4]. In this experiment they measured the momentum distribution of a highly collimated monoenergetic beam of sodium atoms scattered by a plane standing light wave. As an atom passes through the light field, momentum exchanges occur between the light field and the atom in multiples of the photon momentum. The dipole force on the atom results from the momentum exchanged by absorption and stimulated emission of photon pairs. Thus the projection of this momentum along the laser axis is quantized in integral multiples of $2\hbar k$. In the absence of spontaneous emission, that is, for sufficiently detuned atoms, the output in the far field of the scattered atoms consists of several sharply defined peaks. This distribution may be viewed as atomic diffraction of the atoms due to scattering of the atoms from a phase grating formed by the light intensity varying with spatial period $\lambda/2$. As one tunes closer to resonance, the spontaneous emission becomes important. The recoil imparted to the atom by a spontaneously emitted photon occurs in a random direction so that its momentum component in the direction of the standing wave can range from $-\hbar k$ to $+\hbar k$ [5]. Thus spontaneous emission causes the diffractive peaks to be smeared out. This can be viewed as a loss of coherence between parts of the atom wave which scatter from the in-phase parts of the grating formed by the light field. Whereas previous experiments by Pritchard and co-workers were restricted to the diffractive region [6,7], the recent experiment has been able to probe the transition from the diffractive to the diffusive regime. They tuned the laser field closer to atomic resonance to move from the diffractive into the diffusive region. The experimentally measured momentum distributions were compared with calculations based on a purely diffusive model in which there are assumed to be many spontaneous emissions during the interaction with the field. In this limit the atomic momentum is treated classically and the motion is described by a Fokker-Planck equation [8-10]. This diffusive theory has previously been applied to the standing-wave problem by several authors [11-14]. When applied to the experimental data of Gould *et al.* this model adequately describes the envelopes of the momentum distribution but does not accurately predict details of the deflection profiles except when many spontaneous emissions occur. In the purely diffractive limit a quantum-mechanical description of the momentum transfer processes has been given in [6,7,15]. A more general treatment capable of treating the transition region has been formulated by Tanguy, Reynaud, and Cohen-Tannoudji [12] who derived a set of generalized Bloch equations valid in the Raman-Nath regime. To date computational complexities in solving these equations have prevented direct comparison with experiment. In this paper we present a solution of these equations which enables us to compare the theory with the experimental results of Gould *et al.* in all regions. The method developed is computationally efficient, and allows the action of the optical field to be characterized by a relatively small set of numbers which may then be used to determine its effects on an arbitrary input atomic state, and with arbitrary angular distributions of spontaneous emission.

II. PROBLEM FORMULATION

Consider a beam of two-level atoms in their ground state traveling along the z axis which crosses a transverse-optical standing wave along the x axis. We wish to determine the deflection of the atoms as they traverse the light field.

We denote the detuning between the atomic and optical frequencies by $\delta\omega$ and let $E(x,t)=2E_0\mathcal{G}(t)\cos kx\cos\omega_0 t$ denote the standing-wave electric field encountered in the frame of the moving atoms. This leads to a Rabi frequency $\Omega=\mu E_0/\hbar$ where μ is the atomic dipole moment of the transition. The spontaneous emission of the atoms is described by γ^{-1}, the radiative lifetime of the excited state and $\mathcal{G}(t)$ specifies the amplitude profile of the light field encountered by the atoms.

The total atomic state is specified by a density matrix ρ. We shall write $\rho_{ab}(\xi,\xi')$ and $\tilde{\rho}_{ab}(\eta,\eta')$ for the components of the matrix in the position and momentum representations, respectively. The subscripts denote the internal state of the atom and may be e or g for the excited and ground states, respectively. These are written in terms of the dimensionless variables $\xi=kx=\omega_0 x/c$ and $\eta=p/(2\pi\hbar k)$. With these definitions, the representations are

related via a two-dimensional Fourier transform relationship.

The equations of motion of the density matrix are called the generalized optical Bloch equations [12]. In the Raman-Nath regime, the transverse motion of the atoms during the interaction time with the field is neglected. These equations can be written in matrix form as

$$\frac{\partial \rho}{\partial \tau} = \mathcal{L}(\xi,\xi')\rho , \tag{1}$$

where $\mathcal{L}(\xi,\xi')$ is the matrix

$$\begin{pmatrix} -\Gamma & i\mathcal{G}\cos\xi' & -i\mathcal{G}\cos\xi & 0 \\ i\mathcal{G}\cos\xi' & -(\Gamma/2+2i\Delta) & 0 & -i\mathcal{G}\cos\xi \\ -i\mathcal{G}\cos\xi & 0 & -(\Gamma/2-2i\Delta) & i\mathcal{G}\cos\xi' \\ \Gamma\chi(\xi-\xi') & -i\mathcal{G}\cos\xi & i\mathcal{G}\cos\xi' & 0 \end{pmatrix} . \tag{2}$$

Here $\tau=\Omega t$, $\Delta=\delta\omega/(2\Omega)$, and $\Gamma=\gamma/\Omega$. The term $\Gamma\chi$ describes the transfer of atoms from the excited state to the ground state by spontaneous emission. If the angular distribution of spontaneous emission in the direction of the unit normal vector $\mathbf{n}$ is given by $\phi(\mathbf{n})$, $\chi(\mathbf{u})$ is given by the surface integral

$$\chi(\mathbf{u}) = \int d^2\mathbf{n}\,\phi(\mathbf{n})\exp(-ik\mathbf{n}\cdot\mathbf{u}) , \tag{3}$$

where $\phi(\mathbf{n})$ is normalized so that its integral over the entire sphere is unity [12].

The generalized optical Bloch equations form an initial-value problem with $\rho_{ee}=\rho_{eg}=\rho_{ge}=0$ at $\tau=0$ and $\rho_{gg}(\xi,\xi',0)$ being given by the incoming distribution of the atoms. For each pair of coordinates (ξ,ξ') we have a system of four coupled differential equations to integrate. For most practical problems, the number of points at which $\rho(\xi,\xi',\tau)$ has to be computed is large and so techniques have to be developed to reduce this load.

We first specialize to the situation in which $\mathcal{G}$ is constant, which corresponds to the assumption that the intensity of the light field is constant across its profile. The integration can be performed analytically and the solution expressed as

$$\rho(\xi,\xi',\tau) = \exp[\mathcal{L}(\xi,\xi')\tau](0\,0\,0\,\rho_{gg}(\xi,\xi',0))^t . \tag{4}$$

The main requirement is to limit the number of points at which the matrix exponential is evaluated. This is possible because of three observations. The first is that the solution for an arbitrary initial state $\rho_{gg}(\xi,\xi',0)$ may be derived from the solution with $\rho_{gg}(\xi,\xi',0)=1$, since (4) is local in ξ and ξ'. In the momentum representation, this corresponds to using a δ function for the initial state $\tilde{\rho}_{gg}(\eta,\eta',0)=\delta(\eta)\delta(\eta')$.

Second, using a method similar to that employed by Tanguy, Reynaud, and Cohen-Tannoudji [12] for finding the propagator of the Wigner function in the intermediate regime between the diffractive and diffusive regimes, it may be shown that for this initial state, the diagonal terms of the density matrix for the atoms leaving the interaction region may be written as

$$\tilde{\rho}_{ee} = \sum_r \left[\sum_k \sum_l E_{kl}^{(r)}(\tau)\delta(\eta-(2\pi)^{-1}k)\delta(\eta'-(2\pi)^{-1}l)\right] \circ [\tilde{\chi}^{(r)}(\eta)\delta(\eta-\eta')] , \tag{5}$$

$$\tilde{\rho}_{gg} = \sum_r \left[\sum_k \sum_l G_{kl}^{(r)}(\tau)\delta(\eta-(2\pi)^{-1}k)\delta(\eta'-(2\pi)^{-1}l)\right] \circ [\tilde{\chi}^{(r)}(\eta)\delta(\eta-\eta')] . \tag{6}$$

We use the $\circ$ to denote a convolution and $\tilde{\chi}^{(r)}$ to denote the r-fold self-convolution of the Fourier transform of χ. The coefficients $E_{kl}^{(r)}$ and $G_{kl}^{(r)}$ are independent of χ.

The term in each sum for a particular r refers to those atoms which undergo r spontaneous emissions during the interaction with the field. $\tilde{\chi}^{(r)}(\eta)\delta(\eta-\eta')$ is the momentum spreading imparted to an atom due to the random directions of emission of these spontaneously emitted photons. The discrete momentum transfers due to the coherent processes of absorption and stimulated emission give rise to the array of δ functions at the lattice of points spaced $(2\pi)^{-1}$ apart.

In Eqs. (5) and (6), the angular dependence of the spontaneous emission enters only through the functions $\tilde{\chi}^{(r)}$. So if we can calculate $E_{kl}^{(r)}$ and $G_{kl}^{(r)}$, these will enable us to find $\tilde{\rho}_{ee}$ and $\tilde{\rho}_{gg}$ for any angular dependence of the spontaneous emission. This leads to the third observation which is that if $\tilde{\chi}$ is chosen to be

$$\tilde{\chi}(\eta) = \delta(\eta-\alpha) \tag{7}$$

then $\tilde{\chi}^{(r)}(\eta)$ is easy to evaluate and $\tilde{\rho}_{ee}$ and $\tilde{\rho}_{gg}$ consist only of δ functions whose areas give the desired values of $E_{kl}^{(r)}$ and $G_{kl}^{(r)}$ directly. The δ function associated with the triple (k,l,r) is found at

$$\eta=(2\pi)^{-1}k+r\alpha,\quad \eta'=(2\pi)^{-1}l+r\alpha . \tag{8}$$

Thus in summary, we use the artifice of choosing the function given by (7) to obtain a numerical solution for ρ_{ee} and ρ_{gg} using (4) and the initial state $\rho_{gg}(\xi,\xi',0)=1$. If we choose α to be a submultiple of $(2\pi)^{-1}$, a fast Fourier transform gives $\tilde{\rho}_{ee}$ and $\tilde{\rho}_{gg}$ only at those positions in the (η,η') plane given by (8). This gives the coefficients $E_{kl}^{(r)}$ and $G_{kl}^{(r)}$ which completely characterize the action of the light field, since an arbitrary initial state and angular distribution of spontaneous emission may be treated using a sequence of convolutions.

We now consider the range of values of r, k, and l for which these quantities are required. The average number of spontaneous emissions during an interaction time t is given by

$$\bar{N} = \frac{\Omega^2\gamma t}{4\delta\omega^2+\gamma^2} . \tag{9}$$

For the experimental parameters, the largest value of $\bar{N}$ used was 4.5, so that summing r from 0 to 15 was found to include all non-negligible terms. The values of k and l

TABLE I. Experimental and simulation parameters. In all scans, $\gamma = 2\pi \times 10$ MHz and $t = 4.71/\gamma$.

Scan	$\delta\omega$	Ω	$\bar{N}$	s	τ	Δ	Γ
(a)	0	2.36γ	4.5	1.00	13.93	0	0.424
(b)	4.0γ	3.34γ	1.2	1.02	19.33	0.611	0.305
(c)	8.0γ	3.34γ	0.4	1.08	18.26	1.293	0.323

need to cover the range of momenta that can be imparted to the atoms. Again for the experimental parameters it was sufficient to use a 64×64 point grid which allows for momentum transfers up to $32\hbar k$. The interaction with the field is thus characterized completely by $64\times64\times16$ quantities. If we make use of the symmetries in the problem, this is further reduced by a factor of 2.

The quantity measured experimentally is the probability of detecting atoms with different momenta at some distance following the interaction with the field. Any atoms leaving the field in the excited state will spontaneously emit on the way to the detector, changing their momentum due to the recoil. The density matrix for the atoms detected is

$$\tilde{\rho}(\eta,\eta') = \tilde{\rho}_{gg}(\eta,\eta') + \tilde{\rho}_{ee}(\eta,\eta') \circ [\tilde{\chi}(\eta)\delta(\eta-\eta')] . \quad (10)$$

The measured probability density is $\tilde{\rho}(\eta,\eta)$.

III. RESULTS

The experimental results of Gould *et al.* are for a monoenergetic, highly collimated atomic sodium beam crossing a circularly polarized standing-wave laser field with a Gaussian intensity profile. The angular distribution of spontaneous emission for this polarization is given by [10]

$$\phi(\mathbf{n}) = \frac{3}{16\pi}(1+\cos^2\theta) , \quad (11)$$

where θ is the angle between the direction of the spontaneous emission and propagation direction of the laser. The experimental parameters are shown in Table I for three scans, where t is the time taken for the atoms to travel between the $1/e^2$ intensity points of the light field.

In the simulations, there are three adjustable parameters Δ, Γ, and τ, which correspond to the normalized detuning, damping, and interaction time, respectively. Since the simulations use a rectangular rather than a Gaussian beam profile for the light field, we need to define an effective interaction time and Rabi frequency. The effective interaction time used is $\sqrt{\pi/2}t$, which gives the correct result in the case when spontaneous emission may be neglected [6]. If we use a Rabi frequency corresponding to the maximum light intensity, we find that there is moderately good agreement with the experimental results, but the fit to the relative heights of the sharp diffractive peaks may be much improved by adjusting the effective Rabi frequency slightly. If we consider the matrix (2) without the term $\Gamma\chi(\xi-\xi')$, it is possible to write a modified Schrödinger equation equivalent to Eq. (1) with a non-Hermitian effective Hamiltonian. This may be used to calculate efficiently the structure of the diffractive peaks alone [corresponding to the term with $r=0$ in Eq. (6)] for a variety of parameter values. This was used to determine the amount by which the Rabi frequency should be scaled. In the column labeled s in Table I, the scaling factor applied is tabulated, and the subsequent columns list the values of the resulting normalized variables used in the simulations. With this scale factor, we replace Ω by Ω/s in all the definitions of the normalized variables given above. Given the 5% uncertainty in the laser intensity [4] and the nonrectangular beam profile this adjustment appears to be reasonable. The input beam was taken to have a full width at half maximum of $1.2\hbar k$.

In Figs. 1–3, the simulation results (dashed line) are superimposed upon the experimental results (solid line). Both simulation and experimental results have been normalized to give an area of unity under the graphs.

Figure 4 shows how the simulation result for scan (a)

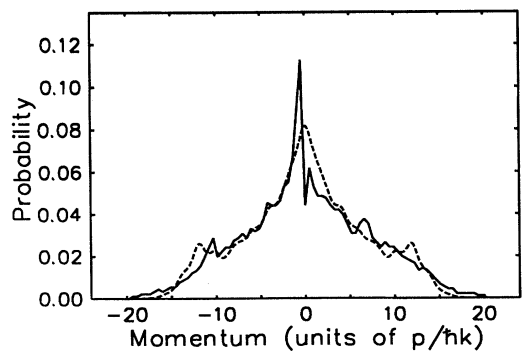

FIG. 1. Comparison of experimental data (solid line) and simulation results (dashed line) for scan (a) of Table I, $\bar{N}=4.5$.

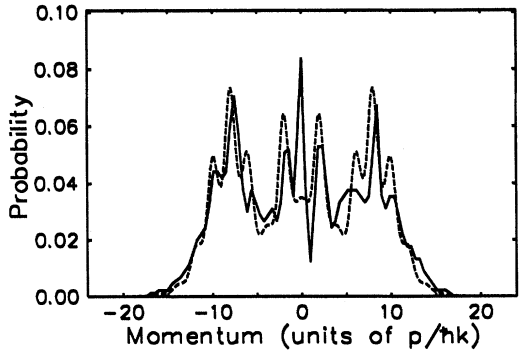

FIG. 2. Comparison of experimental data (solid line) and simulation results (dashed line) for scan (b) of Table I, $\bar{N}=1.2$.

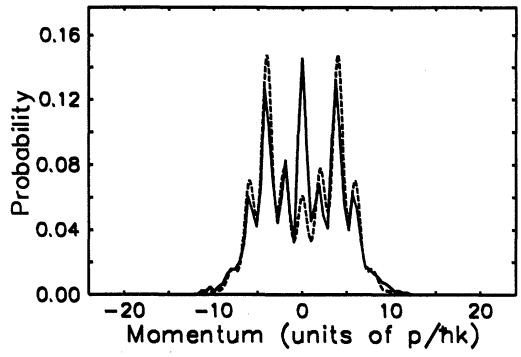

FIG. 3. Comparison of experimental data (solid line) and simulation results (dashed line) for scan (c) of Table I, $\bar{N}=0.4$.

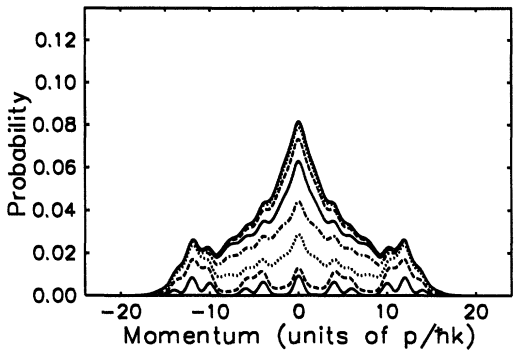

FIG. 4. Partial sums for the simulation of scan (a) in Table I. Starting from the bottom, successive curves include the effects of atoms that have undergone zero, one or fewer, two or fewer, etc., spontaneous emissions on the way to the detector.

was obtained. The series of graphs show a sequence of partial sums monotonically converging to the final result. The lowest solid curve represents those atoms which do not undergo any spontaneous emissions corresponding to the $r=0$ term in Eq. (6) which are responsible for the sharp diffractive peaks. We note that this curve is different from the result of neglecting spontaneous emission completely due to the presence of terms involving Γ on the diagonal of matrix (2). Each successive curve in Fig. 4 shows the result of adding the effects of those atoms undergoing one more spontaneous emission before detection. The curve involving n or fewer decays corresponds to terms with $r \leq n$ in Eq. (6) and with $r \leq n-1$ in Eq. (5). Due to the effects of multiple convolutions with the distribution of recoil momentum, these tend to be smooth and give the diffusive structure. In scan (a), the diffractive component is only a small part of the total, whereas in the corresponding set of graphs for scan (c) the diffractive part is the dominant contribution to the result.

Agreement is quite good in all cases, except for the height of the central peak which represents those atoms which are undeflected by the standing wave. In each case the experimental result of this peak exceeds the theoretical prediction. This may indicate that approximately 5% of the atoms were not prepared in the correct initial state and were unaffected by the light field. The state preparation for the experiment is described by Gould *et al.* [16]. An approximate indication of the size of systematic effects in the experimental data is the degree of asymmetry in the profiles.

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