Quantum scattering of a two-level atom in the limit of large detuning

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In this paper we investigate the scattering of a two-level atom in a traveling or standing wave in the limit of large detuning. We show that these two systems are examples of nontrivial motion which is straightforward to treat using the unified scattering formalism of Tanguy and co-workers [J. Phys. B **17**, 4623 (1984)]. This enables us to compare the diffractive and diffusive approximations with the exact solution of the effective master equation. Our analysis is fully quantum mechanical and in our numerical treatment of the effective master equation we are able to include spontaneous emission to all orders.We find that whereas the diffractive approximation correctly describes scattering from a traveling and a standing wave for short interaction times, the diffusive approximation cannot account for the persistence of diffractive structure for the case of the standing wave. To get good agreement we use an approximation which incorporates both diffractive and diffusive effects.

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I. INTRODUCTION

Atomic optics has a long history that dates back to Maxwell [1], who was the first to show theoretically that electromagnetic waves carry momentum. Before the 1970s a few classic experiments had been done which showed that the mechanical action of light on neutral atoms could lead to significant effects [2,3], but it was not until the development of tunable dye lasers that the resonant light forces on atoms were large enough to allow measurements of the scatter of atoms off light fields [4]. The first scattering experiments were done by Bernhardt and co-workers [5,6] using a traveling-wave light field and Arimondo and co-workers [7] who scattered atoms off a standing wave. Since these early experiments a thorough experimental investigation of the range of scattering regimes has been pursued by Pritchard and co-workers [8–10].

The large number of parameters and the resulting range of physical behavior present a challenge to the theorist trying to model the effective light-atom interaction. There have evolved a number of theoretical methods able to describe the motion of atoms in various regimes. Early theoretical treatments usually assumed that spontaneous emission could be neglected [11]. Reference [12] gives a good review of the range of techniques used to include the force due to spontaneous emission. To a certain extent these approaches were unified by the work of Cook [13], who derived a complete set of differential-difference equations for the atomic Wigner functions. When the state of the atoms was semiclassical in the sense that the Wigner functions were smooth over momentum increments of order $\hbar k$, then the equations reduced to a system of differential equations and in some cases could be reduced further to a single Fokker-Planck equation.

However the assumptions which led to the general semiclassical equations were not valid under the conditions of atomic scattering experiments. For these experiments the atomic-beam momentum is collimated close to the atomic-recoil momentum, and the effects of spontaneous emission range from negligible to cases where it dominates the dynamics [10]. A unified and fully quantum-mechanical theory of atomic scattering was developed by Tanguy and co-workers [14] which provided a framework for general atomic scattering calculations. In their work they stressed the utility of their formalism in treating the transition from diffractive to diffusive scattering. Computational difficulties in integrating the full equations meant that it was not until 1991 that an efficient algorithm for treating them numerically was found by Tan and Walls [15].

It has been pointed out [16] that some scattering experiments have been performed in a regime which allows the development of a fully quantum-mechanical effective master equation that includes the effect of dissipation due to spontaneous emission. This equation was used to show that spontaneous emission leads to a violation of the adiabatic dynamics of the internal state of the atom in the limit of large detuning, and could account for the appearance of momentum exchanges equal to odd multiples of the recoil momentum. In this paper we show that this effective master equation is a nontrivial example of an interaction where the program of Ref. [14] is quite straightforward to carry out. So far the effect of spontaneous emission has been treated perturbatively [14,15], but we will present a numerical scheme which treats spontaneous emission to all orders. Finally we calculate the predictions of this effective master equation in the diffusive limit, and compare the diffusive and diffractive dynamics with a numerical integration of the equations. In Sec. II we derive the effective equations in the large detuning limit. In Sec. III we apply the method of Tanguy and co-workers to investigate the change in dynamics from the diffractive to the diffusive regime.

II. ATOM IN A TRAVELING WAVE: LARGE DETUNING LIMIT

In this section we outline the derivation of the effective master equation in the limit of large detuning. The dy-

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namic variables appropriate for the study of a two-level atom interacting with a classical electromagnetic field are the center-of-mass position and momentum operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$, the internal population inversion operator $\hat{\sigma}_3$, and the internal lowering operator $\hat{\sigma}$ [17]. The coherent coupling between the internal and center-of-mass variables is through the position-dependent Rabi frequency $\Omega(\hat{\mathbf{x}}) = \mathbf{d}\cdot\mathbf{E}(\hat{\mathbf{x}})/\hbar$, where $\mathbf{d}$ is the dipole matrix element for the internal states and $\mathbf{E}(\mathbf{x})$ is the classical electric field vector at position $\mathbf{x}$ [17]. For the important cases of a plane traveling and standing waves

$$\Omega_T(\hat{x}) = \Omega \exp(i\mathbf{k}\cdot\hat{\mathbf{x}}) \;, \tag{2.1a}$$

$$\Omega_S(\hat{x}) = \Omega \cos(\mathbf{k}\cdot\hat{\mathbf{x}}), \tag{2.1b}$$

where $\mathbf{k}$ is the wave vector defining the direction of wave propagation and with magnitude $k = c/\omega$, ω being the wave frequency. In Eqs. (2.1a) and (2.1b) and for the remainder of this paper we denote traveling and standing wave quantities by the subscripts T and S respectively. Without loss of generality Ω is chosen to be real.

There is also an incoherent coupling via the process of spontaneous emission. The starting point for our calculations is the master equation for a two-level atom interacting with a classical field and with the vacuum field modes

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}\left[\hat{H},\hat{\rho}\right] - \gamma\mathcal{L}\hat{\rho}. \tag{2.2}$$

The Hamiltonian $\hat{H}$ generates the coherent dynamics for the center-of-mass and internal states of the atom and is given by

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{\hbar\Delta}{2}\hat{\sigma}_3 - \hbar(\Omega(\hat{\mathbf{x}})\hat{\sigma}^\dagger + \Omega(\hat{\mathbf{x}})^\dagger\hat{\sigma}) \;, \tag{2.3}$$

where Δ is the detuning between the classical field and atomic transition. The incoherent evolution is determined by the spontaneous emission rate γ and the superoperator $\mathcal{L}$. $\mathcal{L}$ describes the twofold effect of a spontaneous emission event: the atom makes a transition from its internal excited state to its ground state, and the spontaneously emitted photon changes its center-of-mass momentum by an amount $\hbar k\mathbf{n}$. The direction of the emitted photon $\mathbf{n}$ is random and has the distribution function [17]

$$\phi(\mathbf{n}) = \frac{3}{8\pi}\left(1 - \frac{(\mathbf{dn})^2}{\mathbf{d}^2}\right). \tag{2.4}$$

$\mathcal{L}$ is given by

$$\mathcal{L}\hat{\rho} = \frac{1}{2}\left(\hat{\sigma}^\dagger\hat{\sigma}\hat{\rho} + \hat{\rho}\hat{\sigma}^\dagger\hat{\sigma} - 2\hat{\sigma}\mathcal{N}\hat{\rho}\hat{\sigma}^\dagger\right), \tag{2.5}$$

and $\mathcal{N}$ is the superoperator describing the effect of a spontaneous emission on the momentum of the atom [17]

$$\mathcal{N}\hat{\rho} = \int d\mathbf{n}\phi(\mathbf{n})\exp(ik\mathbf{n}\cdot\hat{\mathbf{x}})\hat{\rho}\exp(-ik\mathbf{n}\cdot\hat{\mathbf{x}}) \;. \tag{2.6}$$

In the limit that the detuning Δ is much larger than the Rabi frequency Ω and the spontaneous emission rate γ, we can derive the effective master equation (see Appendix)

$$\begin{aligned}\frac{d\hat{\rho}}{dt} = &-\frac{i}{\hbar}\left[\hat{H}_0,\hat{\rho}\right] - \gamma\mathcal{L}\hat{\rho} \\ &+\frac{i}{\Delta}\left[\Omega(\hat{\mathbf{x}})\hat{\sigma}^\dagger, \left(1 - i\frac{\gamma}{\Delta}\mathcal{L}\right)^{-1}\left[\Omega(\hat{\mathbf{x}})^\dagger\hat{\sigma},\hat{\rho}\right]\right] \\ &-\frac{i}{\Delta}\left[\Omega(\hat{\mathbf{x}})^\dagger\hat{\sigma}, \left(1 + i\frac{\gamma}{\Delta}\mathcal{L}\right)^{-1}\left[\Omega(\hat{\mathbf{x}})\hat{\sigma}^\dagger,\hat{\rho}\right]\right],\end{aligned} \tag{2.7}$$

where $\hat{H}_0$ is the free Hamiltonian

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{\hbar\Delta}{2}\hat{\sigma}_3. \tag{2.8}$$

To derive Eq. (2.7) the internal atomic operators $\hat{\sigma}$ and $\hat{\sigma}^\dagger$ are transformed to a frame rotating at frequency Δ and a coarse-graining procedure employed to eliminate dynamics occurring with frequencies of order Δ. Explicit expressions for the inverse superoperators $(1 \pm i\gamma\mathcal{L}/\Delta)^{-1}$ are given in the Appendix.

Denoting the internal ground and excited states by $|a\rangle$ and $|b\rangle$, the evolution of the reduced center-of-mass density operators $\hat{\rho}_a = \langle a|\hat{\rho}|a\rangle$ and $\hat{\rho}_b = \langle b|\hat{\rho}|b\rangle$ is given by the coupled equations

$$\frac{d\hat{\rho}_a}{dt} = -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2m} + \frac{\hbar|\Omega(\hat{\mathbf{x}})|^2}{\Delta|\nu|^2},\hat{\rho}_a\right] + \gamma\mathcal{N}\hat{\rho}_b - \frac{\gamma}{2\Delta^2|\nu|^2}\left[\{|\Omega(\hat{\mathbf{x}})|^2,\hat{\rho}_a\} - 2\Omega(\hat{\mathbf{x}})^\dagger\hat{\rho}_b\Omega(\hat{\mathbf{x}})\right] \;, \tag{2.9a}$$

$$\frac{d\hat{\rho}_b}{dt} = -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2m} - \frac{\hbar|\Omega(\hat{\mathbf{x}})|^2}{\Delta|\nu|^2},\hat{\rho}_b\right] - \gamma\hat{\rho}_b - \frac{\gamma}{2\Delta^2|\nu|^2}\left[\{|\Omega(\hat{\mathbf{x}})|^2,\hat{\rho}_b\} - 2\Omega(\hat{\mathbf{x}})\hat{\rho}_a\Omega(\hat{\mathbf{x}})^\dagger\right], \tag{2.9b}$$

where $\nu = 1 - i\gamma/2\Delta$ and $\{\ ,\ \}$ denotes the anticommutator. We see that in the limit of large detuning the reduced density operators $\hat{\rho}_a$ and $\hat{\rho}_b$ have been decoupled from the off-diagonal operator $\langle a|\hat{\rho}|b\rangle$. Equations (2.7), (2.9a), and (2.9b) differ slightly from those proposed in Ref. [16]. The most obvious difference is that these are operator equations, while the previous equation was derived in the position representation. In addition, our equations recover the exact population densities in the steady state, whereas the effective equation in Ref. [16] does not.

When the spontaneous emission rate γ is set to zero we recover the well known equations for a two-level atom in the large detuning limit [18]. Without noise due to spontaneous emission the internal states are constants of the motion and the reduced density operators $\hat{\rho}_a$ and $\hat{\rho}_b$ satisfy a Hamiltonian evolution in a potential $\hbar|\Omega(x)|^2/\Delta$ ($\hat{\rho}_a$) or $-\hbar|\Omega(x)|^2/\Delta$ ($\hat{\rho}_b$). When the effect of spontaneous emission is included, we see that, as well as the terms describing a transition from the excited state to the ground state when the atom spontaneously emits a photon in a random direction, there are additional terms describing the incoherent emission and absorption of photons at a rate proportional to the magnitude squared of the Rabi frequency.

III. DIFFRACTIVE TO DIFFUSIVE REGIME

In this section we will apply the scattering formalism of Ref. [14] to the equation derived in Sec. II. We will restrict ourselves to the two important cases of a traveling wave and a standing wave. For these two examples we evaluate the propagators for the momentum distribution under the diffractive and diffusive approximations. Finally we present a simple method for numerically integrating the effective scattering equations without approximation.

We are interested in the position and momentum of the atom along the axis defined by the wave vector $\mathbf{k}$. The center-of-mass density operator along this axis is given by $\hat{\rho}_{\mathbf{k}} = Tr(\hat{\rho}_a + \hat{\rho}_b)$, where the trace is taken over states with a position orthogonal to $\mathbf{k}$. In Ref. [14] the atomic center-of-mass density operator $\hat{\rho}_{\mathbf{k}}$ was represented by the Wigner function

$$W(x,p) = \frac{1}{2\pi\hbar}\int du \exp\left(-\frac{ipu}{\hbar}\right) F(x,u), \tag{3.1}$$

where $F(x,u) = \langle x - u/2|\hat{\rho}_{\mathbf{k}}|x + u/2\rangle$, and x is the position along the axis defined by $\mathbf{k}$. In the Raman-Nath regime we assume that the position of the atom does not change during the interaction with the light field. The equations of motion for the states $\hat{\rho}_a$ and $\hat{\rho}_b$ are linear and local in the position representation. Thus the dynamics of the Fourier transform of the Wigner function is determined by a linear propagator. It follows that for an atom initially in the ground state the "in" and "out" states are proportional. That is

$$F_{\text{out}}(x,u) = L(x,u,T)F_{\text{in}}(x,u), \tag{3.2}$$

where T is the interaction time. The "in" and "out" Wigner functions are therefore related by the convolution integral

$$W_{\text{out}}(x,p) = \int d\bar{p} G(x,\bar{p},T) W_{\text{in}}(x,p-\bar{p}), \tag{3.3}$$

where the Wigner function propagator $G(x,\bar{p},T)$ is given by the Fourier transform

$$G(x,\bar{p},T) = \frac{1}{2\pi\hbar}\int du \exp\left(-\frac{i\bar{p}u}{\hbar}\right) L(x,u,T). \tag{3.4}$$

The Wigner function is not a measurable quantity, but rather it is the output momentum distribution

$$P_{\text{out}}(p) = \int dx W_{\text{out}}(x,p), \tag{3.5}$$

which is measured in scattering experiments. Here p is the momentum along the axis defined by $\mathbf{k}$. It is typically the case that in atomic scattering experiments the width in position of the atomic beam is large compared to the wavelength of the scattering field. This means that we can regard the "in" Wigner function as independent of position, the "in" and "out" momentum distributions are related by the convolution

$$P_{\text{out}}(p) = \int d\bar{p}\, G(\bar{p},T) P_{\text{in}}(p-\bar{p}), \tag{3.6}$$

and $G(\bar{p},T)$ is the Green's function averaged over an optical wavelength

$$G(\bar{p},T) = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} dx\, G(x,\bar{p},T). \tag{3.7}$$

Thus $G(\bar{p},T)$ is the probability of absorbing momentum $\bar{p}$ in the time T.

The function $L(x,u,T)$, which depends on the interaction time T, contains all of the information needed to calculate the scattering data, given the atoms initial momentum distribution. Following Tanguy and co-workers we solve for the Laplace transform with respect to time $\tilde{L}(x,u,s)$. We find that for large detuning it is given by

$$\tilde{L}(x,u,s) = \frac{P_1(s)}{P_2(s)}, \tag{3.8}$$

where

$$P_1(s) = s + \gamma - \frac{i}{\Delta}\left(\frac{|\Omega\left(x+\frac{u}{2}\right)|^2}{\nu} - \frac{|\Omega\left(x-\frac{u}{2}\right)|^2}{\nu^*}\right) + \frac{\gamma}{\Delta^2|\nu|^2}\Omega\left(x+\frac{u}{2}\right)\Omega\left(x-\frac{u}{2}\right)^*, \tag{3.9a}$$

$$P_2(s) = \left[s + \frac{i}{\Delta}\left(\frac{|\Omega\left(x+\frac{u}{2}\right)|^2}{\nu^*} - \frac{|\Omega\left(x-\frac{u}{2}\right)|^2}{\nu}\right)\right]\left[s + \gamma - \frac{i}{\Delta}\left(\frac{|\Omega\left(x+\frac{u}{2}\right)|^2}{\nu} - \frac{|\Omega\left(x-\frac{u}{2}\right)|^2}{\nu^*}\right)\right]$$
$$-\frac{\gamma^2}{\Delta^2|\nu|^2}\Omega\left(x+\frac{u}{2}\right)\Omega\left(x-\frac{u}{2}\right)^*\left(\mathcal{N}(u) + \frac{\Omega\left(x-\frac{u}{2}\right)\Omega\left(x+\frac{u}{2}\right)^*}{\Delta^2|\nu|^2}\right). \tag{3.9b}$$

The function $\mathcal{N}(x)$ describes the action of $\mathcal{N}$ in the position representation through the identity $\langle x_1|\mathrm{Tr}(\mathcal{N}\hat{\rho})|x_2\rangle = \mathcal{N}(x_1 - x_2)\langle x_1|\mathrm{Tr}(\hat{\rho})|x_2\rangle$, the trace being taken over states with position orthogonal to $\mathbf{k}$, and is given by

$$\mathcal{N}(x) = \frac{3}{2}\left[\sin\theta\frac{\sin(kx)}{kx} -(1-3\cos^2\theta)\left(\frac{\sin(kx)}{k^2x^2} - \frac{\cos(kx)}{kx}\right)\right], \quad (3.10)$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{d}$. The difficulties in calculating the scattering for arbitrary times are due to the form of $\tilde{L}(x,u,s)$ for the general case. From Eqs. (3.8), (3.9a), and (3.9b) we see that in the limit of large detuning $\tilde{L}(x,u,s)$ is the quotient of a linear function in s and a quadratic function in s. Tanguy and co-workers found that for arbitrary detuning $\tilde{L}(x,u,s)$ was given by the ratio of a cubic to a quartic polynomial in s so that in general the inverse Laplace transform is hard to do. The reduction of the denominator to a quadratic polynomial will prove to be the key to including spontaneous emission to all orders of magnitude.

A. The diffractive approximation

When the interaction time is small enough that we can ignore terms proportional to γ, the motion of the atom is Hamiltonian, and the atom remains in the ground state. This means that there is only one frequency of motion which is reflected in the number of poles of $\tilde{L}(x,u,s)$. For the traveling and standing waves,

$$\tilde{L}_T(x,u,s) = \frac{1}{s}, \quad (3.11)$$

$$\tilde{L}_S(x,u,s) = \frac{1}{s - \frac{i\Omega^2}{\Delta}\sin(2kx)\sin(ku)}. \quad (3.12)$$

It is straightforward to invert the Laplace transform in this case to get

$$L_T(x,u,T) = 1, \quad (3.13)$$

$$L_S(x,u,T) = \exp\left(\frac{i\Omega^2 T}{\Delta}\sin(2kx)\sin(ku)\right). \quad (3.14)$$

The propagators for the Wigner function are

$$G_T(x,p,T) = \delta(p), \quad (3.15)$$

$$G_S(x,p,T) = \sum_{m=-\infty}^{\infty} J_m\left(\frac{\Omega^2 T}{\Delta}\sin(2kx)\right) \times\delta(p - m\hbar k), \quad (3.16)$$

where J_m is the Bessel function of the first kind of order m. To find the propagator of the scattering data we average over a single wavelength to get

$$G_T(p,T) = \delta(p), \quad (3.17)$$

$$G_S(p,T) = \sum_{m=-\infty}^{\infty} J_m\left(\frac{\Omega^2 T}{2\Delta}\right)^2 \delta(p - 2m\hbar k). \quad (3.18)$$

The above result for the momentum propagator in a standing wave, has been derived before assuming that the initial spread in momentum is small compared with the recoil momentum $\hbar k$ [18]. Here we see that this result holds regardless of initial momentum but with the assumption that the width of the atomic beam is large compared with the optical wavelength. When the dynamics is entirely coherent the momentum distribution is unchanged by the traveling wave. In the case of scattering off a standing wave, the change in momentum is always an even multiple of $\hbar k$ [18]. If the initial momentum spread is small compared with $\hbar k$, then the outgoing distribution shows structure on two scales. First there are peaks at even multiples of the recoil momentum. Second on a larger momentum scale there is a slowly varying envelope given by

$$E(\wp) = J_\wp\left(\frac{\Omega^2 T}{2\Delta}\right)^2, \quad (3.19)$$

where $\wp = p/2\hbar k$ denotes the momentum expressed in units of twice the photon momentum. This envelope is localized within the region $|\wp| < \wp_{\max}$, $\wp_{\max} = \Omega^2 T/2\Delta$. For $|\wp| \ll \wp_{\max}$ it has been shown [19] that the envelope shows oscillations reminiscent of Jaynes-Cummings revivals [20]. Using the Airy function approximation for Bessel functions of large integer orders [21], we can derive the following approximation valid in the region $\wp \approx \wp_{\max}$:

$$E(\wp) \approx \left[\frac{4\zeta(z)}{1-z^2}\right]^{1/2} \frac{[\mathrm{Ai}(\wp^{\frac{2}{3}}\zeta(z))]^2}{\wp^{\frac{2}{3}}}, \quad (3.20)$$

where $\mathrm{Ai}(x)$ is the Airy function, $z = \wp/\wp_{\max}$, and the function $\zeta(z)$ is given by

$$\frac{2}{3}\zeta(z)^{\frac{3}{2}} = \ln\left(\frac{1-\sqrt{1-z}}{z}\right) - \sqrt{1-z^2}, \quad z \le 1 \quad (3.21a)$$

$$\frac{2}{3}[-\zeta(z)]^{\frac{3}{2}} = \sqrt{z^2-1} - \arccos\left(\frac{1}{z}\right), \quad z \ge 1. \quad (3.21b)$$

Near $\wp_{\max}$ the behavior of the scattering envelope is dominated by the Airy function. Thus it exhibits a slow oscillation for $|\wp| < \wp_{\max}$ and a rapid decay when $|\wp| > \wp_{\max}$.

B. The diffusive approximation

As we have noted above, the general model for motion in the Raman-Nath regime predicts that $\tilde{L}(x,u,s)$ is the ratio of a cubic to a quartic polynomial in s. This means that there can be up to four different frequencies for the general motion corresponding to the four poles of $\tilde{L}(x,u,s)$ in the complex s plane. When looking at the long time behavior of the atom we assume that the three fastest processes have been damped out and only the slowest one remains. The dynamics of the atom is therefore determined by the pole of $\tilde{L}(x,u,s)$ with the largest real part.

It is difficult to evaluate the propagator for the momentum distribution directly. As a simplification we note that the convolution integral equation (3.6) is more naturally evaluated as a Fourier transform

$$P_{\rm out}(p) = \int_{-\infty}^{\infty} du \exp\left(\frac{ipu}{\hbar}\right) L(u,T)\tilde{P}_{\rm in}(u). \quad (3.22)$$

Here

$$L(u,T) = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} dx L(x,u,T), \quad (3.23)$$

and $\tilde{P}_{in}(u)$ is the Fourier transform of the incoming momentum distribution. In the diffusive regime the function $L(x,u,T)$ is approximated by the Gaussian [14]

$$L(x,u,T) = \exp\left(\frac{iF(x)u}{\hbar}T - \frac{D(x)u^2}{\hbar^2}T\right), \quad (3.24)$$

where

$$F(x) = \frac{\hbar}{i}\frac{\partial s_+}{\partial u}, \quad (3.25)$$

$$D(x) = \frac{1}{2}\left(\frac{\hbar}{i}\right)^2 \frac{\partial^2 s_+}{\partial u^2}, \quad (3.26)$$

and s_+ is the pole of $\tilde{L}(x,u,s)$ with the largest real part. We expect this to be a good approximation to $L(x,u,T)$ when u is small, and thus to correctly describe the scattered momentum distribution for large deflections. We would expect this approximation to break down for small deflections. From Eq. (3.4) we see that approximation (3.24) implies that the propagator satisfies a Fokker-Planck equation [22] in momentum where $F(x)$ is the position-dependent force and $D(x)$ is the diffusion coefficient. Since $\tilde{L}(x,u,s)$ reduces to the ratio of a linear polynomial to a quadratic it is straightforward to find the pole with the largest real part for any functional form of the Rabi frequency. For the traveling wave,

$$F_T = \hbar k\gamma \frac{\Omega^2}{\Delta^2 + \frac{\gamma^2}{4} + 2\Omega^2}, \quad (3.27a)$$

$$D_{1T} = \frac{(\hbar k)^2\gamma}{2}\frac{\Omega^2\sigma}{\Delta^2 + \frac{\gamma^2}{4} + 2\Omega^2}, \quad (3.27b)$$

$$D_{2T} = \frac{(\hbar k)^2\gamma}{2}\frac{\Omega^2}{\Delta^2 + \frac{\gamma^2}{4} + 2\Omega^2} \times \left\{1 - 2(\Delta^2 + \gamma^2/4)\frac{\Omega^2}{[\Delta^2 + \frac{\gamma^2}{4} + 2\Omega^2]^2}\right\}, \quad (3.27c)$$

and for a standing wave,

$$F_S(x) = \hbar k\Delta \frac{\Omega^2 \sin(2kx)}{\Delta^2 + \frac{\gamma^2}{4} + 2\Omega^2\cos^2(kx)}, \quad (3.28a)$$

$$D_{1S}(x) = \frac{(\hbar k)^2}{2}\frac{\gamma\sigma\Omega^2\cos^2(kx)}{\Delta^2 + \frac{\gamma^2}{4} + 2\Omega^2\cos^2(kx)}, \quad (3.28b)$$

$$D_{2S}(x) = \frac{(\hbar k)^2}{2}\frac{\Omega^2 \sin^2(kx)}{\gamma(\Delta^2 + \frac{\gamma^2}{4} + 2\Omega^2\cos^2(kx))} \times \left\{8\Omega^2\cos^2(kx) + \gamma^2 - \frac{2\Delta^2\Omega^2\cos^2(kx)(4\Delta^2+\gamma^2)}{[\Delta^2 + \frac{\gamma^2}{4} + 2\Omega^2\cos^2(kx)]^2}\right\}. \quad (3.28c)$$

In the above expressions D_1 is the spontaneous diffusion coefficient and D_2 is the induced diffusion coefficient [13]. The full diffusion term D is given by the sum $D_1 + D_2$. The term σ describes the distribution in momentum of the spontaneously emitted photons and is given by

$$\sigma = \frac{2}{5}\left(1 - \frac{\cos^2\theta}{2}\right). \quad (3.29)$$

Diffusive approximations have often been used in the study of the resonant interaction between light and matter [23,14,13]. Equations (3.27a), (3.27b), (3.28a), and (3.28b) correspond precisely to the the expressions given in [13]. Both induced diffusion coefficients differ slightly from those derived in Ref. [13], the deviations being small and of order Ω^2/Δ^2 or γ^2/Δ^2.

At this stage we can see the effect of spontaneous emission on the dynamics of an atom scattered by a traveling wave. The diffusive approximation predicts that the disruption to coherent dynamics gives rise to a small net force in the direction of $\mathbf{k}$.

C. Exact solution

When the interaction time T is long enough we can no longer neglect spontaneous emission terms. We can estimate the order of T for which this is so. The rate of spontaneous emission is given by γw, where w is the probability of the atom being in the excited state. For an atom initially in the ground state and when the detuning is large compared to the Rabi frequency and the spontaneous emission rate, $w \approx \Omega^2/\Delta^2$. So the time for one spontaneous emission is approximately $\tau = \Delta^2/(\gamma\Omega^2)$. When $T \ll \tau$ we expect the diffractive approximation to hold. When $T \gg \tau$ we expect the diffusive approximation to hold and when $T \approx \tau$ we are in the intermediate regime. In the intermediate regime we expect to see a mixture of diffractive and diffusive effects, and we must use the exact expression for $L(x,u,T)$. Tan and Walls [15] numerically solved the scattering equations for arbitrary detunings by adding contributions to the propagator due to successively greater numbers of spontaneous emissions. The simplification of the interaction in the limit of large detuning enables one to numerically integrate the equations including all orders of spontaneous emission.

Since $L(x,u,T)$ is the ratio of a linear to a quadratic polynomial in the limit of large detuning we can invert the Laplace transform to get

$$L(x,u,t) = \frac{s_+ + a}{s_+ - s_-}\exp(s_+ t) + \frac{s_- + a}{s_- - s_+}\exp(s_- t), \tag{3.30}$$

where $s_\pm$ are the roots of $P_2(s)$ and $P_1(s) = s + a$. The roots are straightforward to evaluate and we find for the traveling wave,

$$a_T(x,u) = \gamma + \frac{\gamma\Omega^2}{\Delta^2|\nu|^2}[1 + \exp(iku)] \ , \tag{3.31a}$$

$$\begin{aligned} s_T(x,u)_\pm = &-\frac{\gamma}{2}\left(1 + \frac{2\Omega^2}{\Delta^2|\nu|^2}\right) \\ &\pm\left[\gamma^2\left(1 + \frac{2|\Omega|^2}{\Delta^2|\nu|^2}\right)^2 \right. \\ &\left. -\frac{\gamma^2\Omega^2}{\Delta^2|\nu|^2}[1 - \mathcal{N}(u)\exp(iku)]\right]^{1/2} , \end{aligned} \tag{3.31b}$$

and for a standing wave,

$$\begin{aligned} a_S(x,u) = \gamma &+ \frac{4i\Omega^2}{\Delta|\nu|^2}\sin(2kx)\sin(ku) \\ &+ \frac{2\gamma\Omega^2}{\Delta^2|\nu|^2}\cos^2(kx)\cos^2\left(\frac{ku}{2}\right), \end{aligned} \tag{3.32a}$$

$$s_S(x,u)_\pm = A(x,u) \pm \frac{1}{2}\sqrt{B(x,u)}, \tag{3.32b}$$

where

$$A(x,u) = -\frac{\gamma}{2}\left(1 + \frac{16\Omega^2}{\Delta^2|\nu|^2}[1 + \cos(2kx)\cos(ku)]\right) , \tag{3.33a}$$

$$\begin{aligned} B(x,u) = \gamma^2 &+ \frac{16\gamma^2\Omega^4}{\Delta^4|\nu|^4}[1 + \cos(2kx)\cos(ku)]^2 \\ &- \frac{4\Omega^4}{\Delta^2|\nu|^2}\sin^2(2kx)\sin^2(ku) \\ &+ \frac{4i\Omega^2}{\Delta|\nu|^2}\sin(2kx)\sin(ku) \\ &+ \frac{2\gamma^2\Omega^2}{\Delta^2|\nu|^2}[\cos(2kx) + \cos(ku)]\mathcal{N}(u) \ . \end{aligned} \tag{3.33b}$$

To find the output momentum distribution for the traveling and standing waves we numerically averaged over position as in Eq. (3.23), and then evaluated Eq. (3.22) using a fast Fourier transform.

In Figs. 1 and 2 we have graphed the scattered momentum distribution calculated from the effective master equation (2.7) together with the predictions of the diffractive and diffusive approximations. In both figures we have taken the incoming momentum distribution to be a Gaussian centered on $p = 0$ with full width at half maximum of $0.7\hbar k$ and $\theta = \pi/2$. In Fig. 1 we have graphed the scattering data for an atom in a traveling wave. We see that as the interaction time T is increased from $T = 0.1\tau$ to $T = 10\tau$ the diffractive approximation diverges from a full integration of the effective master equation. On the other hand, as T increases, predictions from a full integration and from the diffusive approximation appear to converge.

In Fig. 2 we have graphed the scattering data for an atom in a standing wave. For $T = 0.1\tau$ the diffractive approximation is in quite good agreement with a full solution of the quantum-mechanical equations. When $T = \tau$ a full solution displays the peak structure of purely diffractive motion as well as a smooth diffusivelike component. When $T = 10\tau$ we would expect from Fig. 1 that

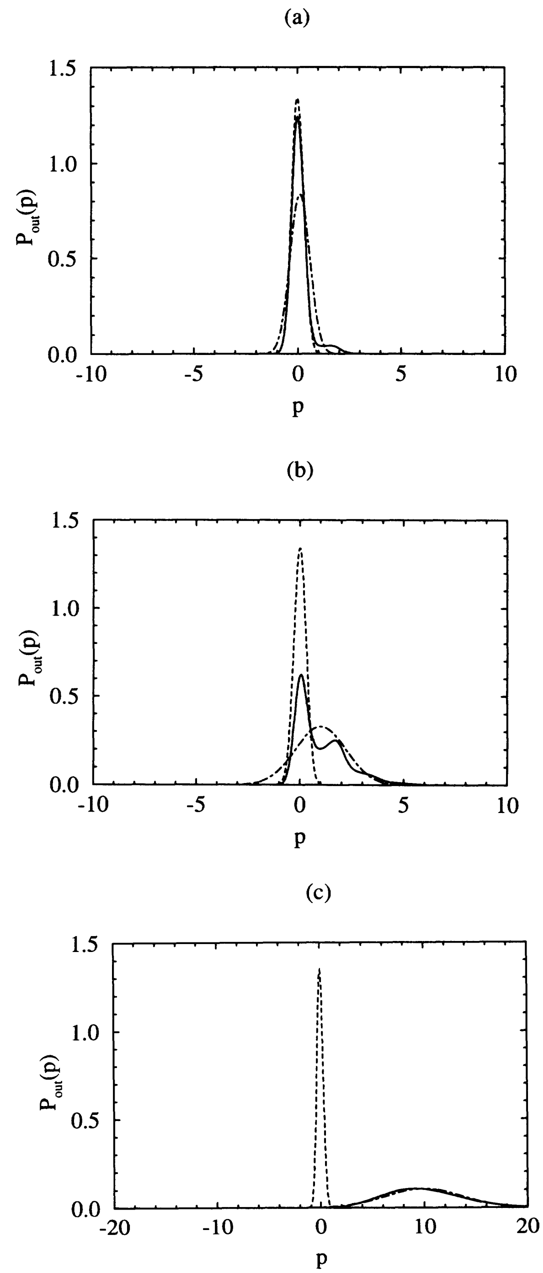

FIG. 1. Scattering data for a traveling wave versus momentum measured in units of $\hbar k$. (a) $T = 0.1\tau$, (b) $T = \tau$, (c) $T = 10\tau$. $\Omega/\Delta = \gamma/\Delta = 0.05$. Solid line, full solution; dashed line, diffractive approximation; dot-dashed line, diffusive approximation.

the momentum distribution should be diffusive in character. However, from Fig. 2(b), we see that there still remains a diffractive component to the outgoing momentum. For small momenta we see peaks due to momentum exchanges in units of $2\hbar k$ as well as oscillations at the wings of the scattering distribution. While it is expected from Sec. III B that the diffusive approximation might fail to account for the structure around $p = 0$, it is surprising that it cannot account for the oscillations in $P_{\rm out}(p)$ near the points of maximum deflection. These oscillations are in fact remnants of the diffractive envelope discussed in Sec. III A. In order to show this we have plotted in Fig. 3 the envelope function given by Eq. (3.20), together with the scattered momentum distribution in the region of maximum positive deflection and for $T = 10\tau$. It is clear that spontaneous emission has smoothed out the diffractive peak structure but has not yet destroyed the large-scale envelope. We are motivated by this to find a new approximation for the standing-wave case which incorporates the diffusive effect of spontaneous emission and the diffractive effect of the coherent evolution. This is accomplished as follows. As for the diffusive approximation we assume that the scattering dynamics is determined by $s(x,u)_+$. Now note that $\Omega^2/\Delta \ll \gamma$ in our numerical examples. Therefore we may approximate $s(x,u)_+$ by a sum of the coherent term

$$s(x,u)_c = \frac{i\Omega^2}{\Delta|\nu|^2}\sin(2kx)\sin(ku), \tag{3.34}$$

and the incoherent term

$$s(x,u)_{inc} = -\frac{\gamma\Omega^2}{2\Delta^2|\nu|^2}\{1+\cos(2kx)\cos(ku) -[\cos(2kx)+\cos(ku)]\mathcal{N}(u)\}. \tag{3.35}$$

Now apply the diffusive approximation to the incoherent term only. After replacing $\cos^2(kx)$ and $\sin^2(kx)$ in the resulting expression by their average 1/2, it is straightforward to evaluate the propagator for the momentum distribution which we find to be

$$G_S(p,T) = \sum_{m=-\infty}^{\infty} J_m\left(\frac{\Omega^2 T}{2\Delta|\nu|^2}\right)^2 g(p-2m\hbar k, T), \tag{3.36}$$

where

$$g(p,T) = \frac{1}{\sqrt{2\pi DT}}\exp\left(-\frac{p^2}{2DT}\right), \tag{3.37a}$$

$$D = \frac{\gamma\Omega^2}{2\Delta^2|\nu|^2}(\sigma+1)\hbar^2k^2. \tag{3.37b}$$

Under this approximation $G_S(p,T)$ has the same form as the diffractive propagator Eq. (3.18) but now the δ func-

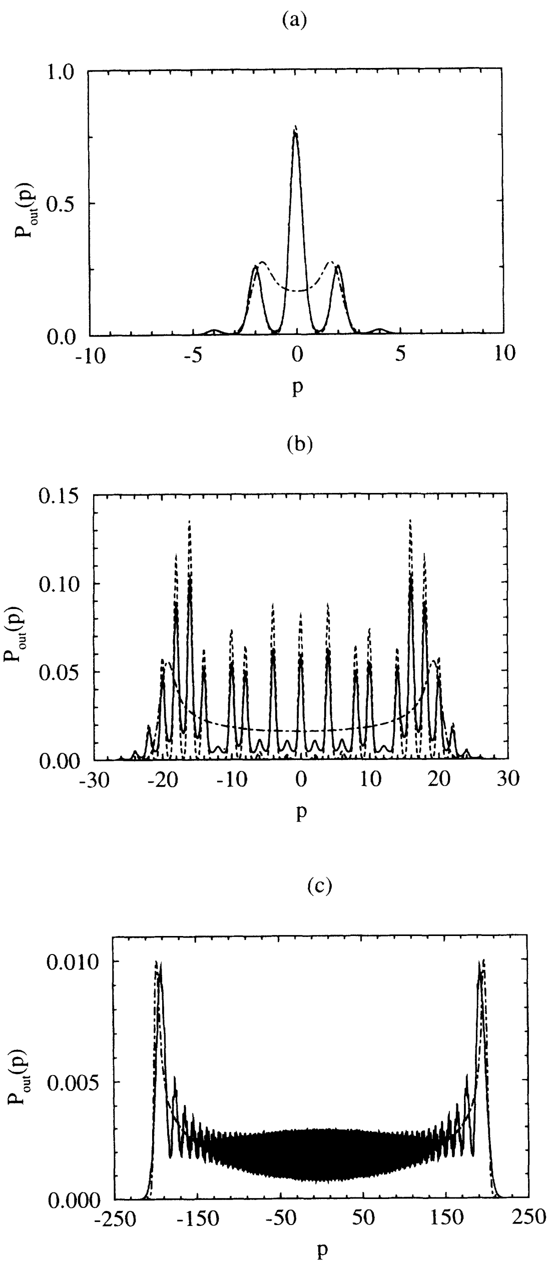

FIG. 2. Scattering data for a standing wave versus momentum measured in units of $\hbar k$. (a) $T = 0.1\tau$, (b) $T = \tau$, (c) $T = 10\tau$. $\Omega/\Delta = \gamma/\Delta = 0.05$. Solid line, full solution; dashed line, diffractive approximation; dot-dashed line, diffusive approximation.

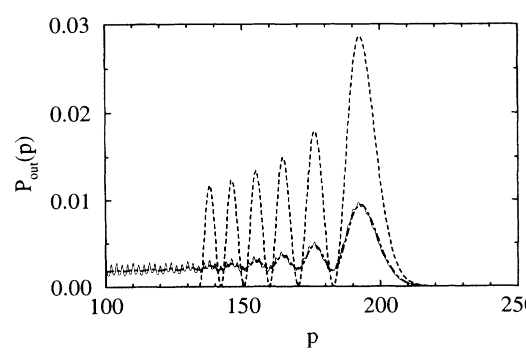

FIG. 3. Scattering data for a standing wave near the region of maximum positive deflection. $T = 10\tau$, $\Omega/\Delta = \gamma/\Delta = 0.05$. Solid line, full solution; dashed line, diffractive envelope; dot-dashed line, intermediate approximation.

tion has been replaced by a slowly diffusing Gaussian. The scattered momentum distribution given by this intermediate approximation at $T = 10\tau$ is given in Fig. 3. We see that there is good agreement with the exact solution.

IV. DISCUSSION

In this paper we have shown that a variant of the master equation first proposed by Kazentsev and co-workers [16] is straightforward to treat within the unified scattering formalism of Ref. [14]. Unlike a previous numerical treatment of the exact master equations, we are able to include spontaneous emission to all orders in our simulations. We have compared the predictions of the diffractive and diffusive approximations for the important cases of the traveling- and the standing-wave electromagentic fields with a full solution of the effective equations. We have found that, while there is good agreement for the case of a traveling wave, the diffusive approximation cannot account for the persistence of diffractive structure when the atom is scattered from a standing wave. This structure can be accounted for using an approximation which incorporates both diffractive and diffusive effects.

APPENDIX

In deriving an effective master equation our aim is to eliminate the dynamics of the internal atomic states occurring at a frequency Δ due to the coherent interaction with the classical electromagnetic field but still retain the slow dynamics due to the incoherent interaction with the quantized vacuum modes.

We start by transforming the density operator $\hat{\rho}$ from the Schrödinger picture to the interaction picture

$$\hat{\rho}_I = \exp\left(-i\frac{\Delta t\hat{\sigma}_3}{2}\right)\hat{\rho}\exp\left(i\frac{\Delta t\hat{\sigma}_3}{2}\right). \tag{A1}$$

$\hat{\rho}_I$ now satisfies the time-dependent master equation

$$\frac{d\hat{\rho}_I}{dt} = -\frac{i}{\hbar}\left[\hat{H}_I(t), \hat{\rho}_I\right] - \gamma\mathcal{L}\hat{\rho}_I, \tag{A2}$$

where $\hat{H}_I(t)$ is the time-dependent Hamiltonian

$$\hat{H}_I(t) = \frac{\hat{\mathbf{p}}^2}{2m} - \hbar[\Omega(\hat{\mathbf{x}})\hat{\sigma}^\dagger \exp(-i\Delta t) + \Omega(\hat{\mathbf{x}})^\dagger\hat{\sigma}\exp(i\Delta t)] \, . \tag{A3}$$

Let T be a time interval large compared to the free oscillation period $2\pi/\Delta$. We eliminate the fast dynamics by averaging $\hat{\rho}_I$ over the time T

$$\langle\hat{\rho}_I(t)\rangle = \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} \hat{\rho}_I(t+\tau)d\tau. \tag{A4}$$

The time-averaged density operator obeys the master equation

$$\frac{d\langle\hat{\rho}_I\rangle}{dt} = -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2m}, \langle\hat{\rho}_I\rangle\right] + i\left[\Omega(\hat{\mathbf{x}})\hat{\sigma}^\dagger, \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} \exp[-i\Delta(t+\tau)]\hat{\rho}_I(t+\tau)d\tau\right] + i\left[\Omega(\hat{\mathbf{x}})^\dagger\hat{\sigma}, \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} \exp[i\Delta(t+\tau)]\hat{\rho}_I(t+\tau)d\tau\right] - \gamma\mathcal{L}\langle\hat{\rho}_I\rangle \, . \tag{A5}$$

If $\Omega \ll \Delta$ then the integrals in the above expression can be estimated by repeated integration by parts. Expanding to lowest order in the small parameter Ω/Δ and neglecting the rapidly oscillating boundary terms, we obtain the following expressions:

$$\frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} \exp[-i\Delta(t+\tau)]\hat{\rho}_I(t+\tau)d\tau \approx \left(1 - i\frac{\gamma}{\Delta}\mathcal{L}\right)^{-1}\frac{1}{\Delta}\left[\Omega(\hat{\mathbf{x}})^\dagger\hat{\sigma}, \langle\hat{\rho}_I\rangle\right], \tag{A6a}$$

$$\frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} \exp[i\Delta(t+\tau)]\hat{\rho}_I(t+\tau)d\tau \approx -\left(1 + i\frac{\gamma}{\Delta}\mathcal{L}\right)^{-1}\frac{1}{\Delta}\left[\Omega(\hat{\mathbf{x}})\hat{\sigma}^\dagger, \langle\hat{\rho}_I\rangle\right]. \tag{A6b}$$

So to lowest order in Ω/Δ the smoothed density operator satisfies

$$\frac{d\langle\hat{\rho}_I\rangle}{dt} = -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{p}}^2}{2m}, \langle\hat{\rho}_I\rangle\right] + \frac{i}{\Delta}\left[\Omega(\hat{\mathbf{x}})\hat{\sigma}^\dagger, \left(1 - i\frac{\gamma}{\Delta}\mathcal{L}\right)^{-1}[\Omega(\hat{\mathbf{x}})^\dagger\hat{\sigma}, \langle\hat{\rho}_I\rangle]\right] - \frac{i}{\Delta}\left[\Omega(\hat{\mathbf{x}})^\dagger\hat{\sigma}, \left(1 + i\frac{\gamma}{\Delta}\mathcal{L}\right)^{-1}[\Omega(\hat{\mathbf{x}})\hat{\sigma}^\dagger, \langle\hat{\rho}_I\rangle]\right] - \gamma\mathcal{L}\langle\hat{\rho}_I\rangle \, . \tag{A7}$$

In order to drop the time averaging brackets in the above expression we require that T be much smaller than the natural lifetime $1/\gamma$. This condition is satisfied if $\gamma \ll \Delta$. Therefore, if $\Omega, \gamma \ll \Delta$, we get Eq. (2.7) after transforming back to the Schrödinger picture .

To derive Eqs. (2.9a) and (2.9b) we need to calculate the inverse superoperator $(1 \pm i\gamma\mathcal{L}/\Delta)^{-1}$. First expand in a Taylor series

$$\left(1 \pm i\frac{\gamma}{\Delta}\mathcal{L}\right)^{-1} = \sum_{n=0}^{\infty}\left(\mp i\frac{\gamma}{\Delta}\right)^{n}\mathcal{L}^{n}. \tag{A8}$$

$\mathcal{L}^n$ has the following action on an arbitrary operator $\hat{A}$:

$$\mathcal{L}^n\hat{A} = \begin{cases} \hat{A}\,, \quad n=0 \\ \left(\frac{1}{2}\right)^{n}\left(\hat{\sigma}\hat{\sigma}^{\dagger}\hat{A}\hat{\sigma}^{\dagger}\hat{\sigma} + \hat{\sigma}^{\dagger}\hat{\sigma}\hat{A}\hat{\sigma}\hat{\sigma}^{\dagger}\right) \\ \qquad +\hat{\sigma}^{\dagger}\hat{\sigma}\hat{A}\hat{\sigma}^{\dagger}\hat{\sigma} - \mathcal{N}\hat{\sigma}\hat{A}\hat{\sigma}^{\dagger}, \quad n \geq 1\,. \end{cases} \tag{A9}$$

Substituting for Eq. (A9) into Eq. (A8) and summing over n we find that $(1 \pm i\gamma\mathcal{L}/\Delta)^{-1}$ has the following action:

$$\begin{aligned}\left(1 \pm i\frac{\gamma}{\Delta}\mathcal{L}\right)^{-1}\hat{A} &= \hat{A} \mp i\frac{\gamma}{2\Delta}\left(1 \pm i\frac{\gamma}{2\Delta}\right)^{-1} \\ &\times\left(\hat{\sigma}\hat{\sigma}^{\dagger}\hat{A}\hat{\sigma}^{\dagger}\hat{\sigma} + \hat{\sigma}^{\dagger}\hat{\sigma}\hat{A}\hat{\sigma}\hat{\sigma}^{\dagger}\right) \\ &\mp i\frac{\gamma}{\Delta}\left(1 \pm i\frac{\gamma}{\Delta}\right)^{-1}\left(\hat{\sigma}^{\dagger}\hat{\sigma}\hat{A}\hat{\sigma}^{\dagger}\hat{\sigma} - \mathcal{N}\hat{\sigma}\hat{A}\hat{\sigma}^{\dagger}\right).\end{aligned} \tag{A10}$$

[1] J. C. Maxwell, *A Treatise on Electricity and Magnetism*, 3rd ed. (Clarendon Press, Oxford, 1982), Vol. 2.
[2] P. N. Lebedev, Ann. Phys. (Paris) **32**, 411 (1910).
[3] O. R. Frish, Z. Phys. **86**, 42 (1933).
[4] A. Ashkin, Phys. Rev. Lett. **25**, 1321 (1970).
[5] A. F. Bernhardt, D. E. Duerre, J. R. Simpson, and L. L. Wood, Appl. Phys. Lett. **25**, 617 (1974).
[6] A. F. Bernhardt, Appl. Phys. **9**, 19 (1976).
[7] E. Arimondo, H. Lew, and T. Oka, Phys. Rev. Lett. **43**, 753 (1979).
[8] P. E. Moskowitz, P. L. Gould, S. R. Atlas, and D. E. Pritchard, Phys. Rev. Lett. **51**, 370 (1983).
[9] P. L. Gould, G. A. Ruff, and D. E. Pritchard, Phys. Rev. Lett. **56**, 827 (1986).
[10] P. L. Gould, P. J. Martin, G. A. Ruff, R. E. Stoner, J. Picque, and D. E. Pritchard, Phys. Rev. A **43**, 585 (1991).
[11] R. J. Cook and A. F. Bernhardt, Phys. Rev. A **18**, 2533 (1981).
[12] A. P. Kazentsev, Usp. Fiz. Nauk **124**, 113 (1978) [Sov. Phys. Usp. **21**, 58 (1978)].
[13] R. J. Cook, Phys. Rev. **22**, 1078 (1980).
[14] C. Tanguy, S. Reynaud, and C. Cohen-Tannoudji, J. Phys. B **17**, 4623 (1984).
[15] S. M. Tan, and D. F. Walls, Phys. Rev. A **44**, R2779 (1991).
[16] A. P. Kazentsev, G. I. Surdutovich, V. P. Yakovlev, and D. O. Chudesnikov, Opt. Commun. **52**, 311 (1985).
[17] A. P. Kazentsev, G. I. Surdutovich, and V. P. Yakovlev, *Mechanical Action of Light on Atoms* (World Scientific, Singapore, 1991).
[18] A. P. Kazentsev, G. I. Surdutovich, and V. P. Yakovlev, Pis'ma Zh. Eksp. Teor. Fiz. **31**, 542 (1980) [JETP Lett. **31**, 509 (1980)].
[19] V. M. Akulin, Fam Le Kien, and W. P. Schleich, Phys. Rev. A **44**, R1462 (1991).
[20] N. B. Narozhny, J. J. Sanchez-Mondragon, and J. H. Eberly, Phys. Rev. A **23**, 236 (1981).
[21] *Handbook of Mathematical Functions*, Natl. Bur. Stand. (U.S.) Appl. Math. Ser. No. 55, edited by M. Abramowitz, and I. A. Stegun (U.S. GPO, Washington, DC, 1965).
[22] C. W. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, New York, 1985).
[23] J. L. Picque, Phys. Rev. A **19**, 1622 (1979).