

Evolution of the velocity distribution of atoms under the action of the bichromatic forceV. I. Romanenko * and L. P. Yatsenko *Institute of Physics of the National Academy of Sciences of Ukraine, Nauky Avenue 46, Kyiv 03680, Ukraine*

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We study numerically the evolution of the velocity distribution of atoms under the action of the bichromatic force. The comparison of the time dependencies of the distribution width and the average acceleration of atoms reveals the correlation of these quantities. We show that the estimation of the momentum diffusion coefficient on the basis of the analogy between the interaction of atoms with the counterpropagating bichromatic waves and the interaction of atoms with the counterpropagating sequences of the π pulses roughly corresponds to the results of numerical calculations. To separate the influence of the momentum diffusion on the evolution of atomic momentum distribution from the influence of the time-dependent Doppler shift, we study the motion of a “heavy” atom, for which the velocity change during the interaction of an atom with the field can be neglected. Provided that the parameters of the atom-field interaction are optimal, we show that the momentum diffusion coefficient is proportional to the intensity of the laser radiation. We used the Monte Carlo wave-function method for the numerical simulation of the atomic motion.

DOI: [10.1103/PhysRevA.103.043104](https://doi.org/10.1103/PhysRevA.103.043104)**I. INTRODUCTION**

The first theoretical study of the light pressure force exerted on atoms in the field of counterpropagating bichromatic waves in 1988 [1] showed that this force can be used to control the motion of atoms. This control is based on the large light pressure force exerted on atoms, which is much larger than the maximal light pressure force F_{rad} in the field of a traveling monochromatic wave, given by the formula [2,3]

$$F_{\text{rad}} = \frac{1}{2} \hbar k \gamma. \quad (1)$$

Here γ is the rate of the spontaneous emission, and k is the wave vector. This fundamental limit was exceeded already in the first observation of the bichromatic force [4]. Later, the light pressure force much greater than F_{rad} was experimentally confirmed [5]. Analytical theory of the bichromatic force was developed in Refs. [6,7], and a review of publications on this topic is given in Ref. [8]. At the same time, momentum diffusion of atoms in the field of counterpropagating bichromatic waves has not been studied so far, in contrast to well-known thorough studies of momentum diffusion of atoms in the field of monochromatic waves [2,9] and momentum diffusion of atoms in the field of π pulses [10].

To describe the evolution of the velocity distribution of atoms under the action of the bichromatic force, we track the time dependence of two statistical characteristics of the distribution. These characteristics are the average velocity \bar{v} of atoms and the standard deviation Δv of the velocity from the average value. We find \bar{v} and Δv from the atomic state vector of each atom using the Monte Carlo wave-function method [11,12]. We show that only at the beginning of the

interaction of the atoms with the field the time evolution of the width Δp of the momentum distribution of the atoms can be described by the diffusionlike dependence $\Delta p = \sqrt{2Dt}$, where D is the momentum diffusion coefficient and t is the atom-field interaction time. Over time, Δp can both increase and decrease.

To separate the influence of momentum diffusion on the evolution of momentum distribution of atoms from the influence of the time-dependent Doppler shift of the atomic frequency, we used an assumption of a “heavy” atom, in which the change of the Doppler shift during the interaction of the atom with the field can be neglected. This allowed us to study the dependencies of the momentum diffusion coefficient on the average velocity of atoms and the momentum diffusion coefficient on the intensity of laser radiation.

The paper is structured as follows. The next section presents the equations that describe the time dependence of the field acting on the atoms and the Hamiltonian of the atom-field interaction. The third section describes the Monte Carlo method for the wave function. In the fourth section, we present the scheme of the numerical calculation. The obtained results are discussed in the fifth section. In the sixth section, we formulate conclusions of the work.

II. ELECTRIC FIELD AND HAMILTONIAN

Consider a two-level atom with the ground $|g\rangle$ and the excited $|e\rangle$ states, which interacts with two counterpropagating bichromatic waves

$$\begin{aligned} \mathbf{E}_p = & \frac{1}{2} \mathbf{e} E_0 \cos \left[(\omega + \delta)t + \frac{\varphi}{2} - kz \right] \\ & + \frac{1}{2} \mathbf{e} E_0 \cos \left[(\omega - \delta)t - \frac{\varphi}{2} - kz \right] \end{aligned} \quad (2)$$

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and

$$\mathbf{E}_m = \frac{1}{2} \mathbf{e} E_0 \cos \left[(\omega + \delta)t - \frac{\varphi}{2} + kz \right] + \frac{1}{2} \mathbf{e} E_0 \cos \left[(\omega - \delta)t + \frac{\varphi}{2} + kz \right], \quad (3)$$

where E_0 is the peak amplitude of the waves, which is assumed to be the same for all waves, \mathbf{e} is the unit polarization vector, and $\omega \pm \delta$ are the carrier frequencies with the mean frequency ω and the difference 2δ .

Here we neglected the difference of the wave vectors $\sim (\delta/\omega)k$; taking it into account leads to a change in the phase difference, which is substantial at a distance of the order $c/\delta \sim 1 \text{ m} \sim (10^6 - 10^7)\lambda$, where λ is the wavelength of electromagnetic radiation. In our model, used in other works [1,4–6,10,13,14], we describe the phase difference between the waves by the terms $\pm\varphi/2$.

The Hamiltonian of an atom in the field

$$\mathbf{E} = \mathbf{E}_p + \mathbf{E}_m \quad (4)$$

has the form

$$H = \frac{\hat{\mathbf{p}}^2}{2M} + \hbar\omega_0 |e\rangle\langle e| - \hat{\mathbf{d}} \cdot \mathbf{E}. \quad (5)$$

Here $\hat{\mathbf{p}}$ is the momentum operator of the atom, M is the atomic mass, ω_0 is the transition frequency ($\hbar\omega_0$ is the energy difference of the states e and g), and $\hat{\mathbf{d}}$ is the dipole momentum operator.

The field Eq. (4) can be written as counterpropagating amplitude-modulated waves:

$$\mathbf{E} = \mathbf{e} E_1 \cos(\omega t - kz) + \mathbf{e} E_2 \cos(\omega t + kz), \quad (6)$$

where

$$E_1 = E_0 \cos \left(\delta t + \frac{1}{2} \varphi \right), \quad (7)$$

$$E_2 = E_0 \cos \left(\delta t - \frac{1}{2} \varphi \right). \quad (8)$$

Here E_0 is the amplitude of the counterpropagating waves. The field Eq. (4) can also be interpreted as a bichromatic standing wave:

$$E = E_0 \cos \left(kz + \frac{\varphi}{2} \right) \cos [(\omega - \delta)t] + E_0 \cos \left(kz - \frac{\varphi}{2} \right) \cos [(\omega + \delta)t], \quad (9)$$

with the amplitude E_0 of the monochromatic components.

III. SCHRÖDINGER EQUATION AND MODELING OF THE STATE VECTOR BY MONTE CARLO WAVE-FUNCTION METHOD

We determine the temporal evolution of the state vector $|\psi\rangle$ from the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle - i\hbar \frac{\gamma}{2} |e\rangle\langle e| |\psi\rangle \quad (10)$$

by the Monte Carlo wave-function method [11,12].

The last term in Eq. (10) describes the spontaneous emission by the atom in the excited state with the rate γ . To reduce the number of equations needed to describe the evolution of the state vector, we assume, as in Ref. [12], that the momentum of the atom along the Oz axis is changed after spontaneous emission by $\pm\hbar k$ or does not change at all (the photon is emitted in the orthogonal to the Oz axis direction).

We seek the state vector in the form

$$|\psi\rangle = c_g(z, t) |g\rangle + c_e(z, t) e^{-i\omega_0 t} |e\rangle. \quad (11)$$

Substituting Eqs. (6) and (11) in Eq. (10), and assuming that the components of the bichromatic waves are symmetrically detuned with respect to the optical transition frequency ω_0 , we find the equations for $c_g(z, t)$ and $c_e(z, t)$ in the rotating-wave approximation [15]:

$$i \frac{\partial}{\partial t} c_g = -\frac{\hbar}{2M} \frac{\partial^2}{\partial z^2} c_g + \frac{1}{2} (V_1 e^{-ikz} + V_2 e^{ikz}) c_e, \quad (12)$$

$$i \frac{\partial}{\partial t} c_e = -\frac{\hbar}{2M} \frac{\partial^2}{\partial z^2} c_e + \frac{1}{2} (V_1 e^{ikz} + V_2 e^{-ikz}) c_g - i \frac{\gamma}{2} c_e. \quad (13)$$

Here V_1 and V_2 are defined by the expressions

$$V_1 = -\frac{1}{\hbar} \langle g | \hat{\mathbf{d}} \cdot \mathbf{e} | e \rangle E_1 = \Omega_R \cos \left(\delta t + \frac{1}{2} \varphi \right), \quad (14)$$

$$V_2 = -\frac{1}{\hbar} \langle g | \hat{\mathbf{d}} \cdot \mathbf{e} | e \rangle E_2 = \Omega_R \cos \left(\delta t - \frac{1}{2} \varphi \right), \quad (15)$$

where $\Omega_R = -\langle g | \hat{\mathbf{d}} \cdot \mathbf{e} | e \rangle E_0 / \hbar$ is the Rabi frequency. To simplify the notations, in Eqs. (12) and (13) and hereinafter, we omit the arguments denoting the dependence of quantities on time and coordinates.

We write c_g and c_e in the forms

$$c_g = \sum_{n=-\infty}^{\infty} b_{g,n} \exp \left(ik_0 z + inkz - i \frac{\hbar k_0^2}{2M} t \right), \quad (16)$$

$$c_e = \sum_{n=-\infty}^{\infty} b_{e,n} \exp \left(ik_0 z + inkz - i \frac{\hbar k_0^2}{2M} t \right), \quad (17)$$

where $k_0 = p_0 / \hbar$, and p_0 is the z component of the initial momentum of the atom along the axis Oz . Time-dependent phases in Eqs. (16) and (17) do not influence the probabilities $b_{g,n}$ and $b_{e,n}$ to find the atom in the states $|g, n\rangle = |g\rangle \otimes |n\rangle$ and $|e, n\rangle = |e\rangle \otimes |n\rangle$.

To obtain the equations for $b_{g,n}$ and $b_{e,n}$, we substitute Eqs. (16) and (17) in Eqs. (12) and (13):

$$\frac{\partial}{\partial t} b_{g,n} = -i \left(n^2 \delta_{\text{rec}} + \frac{n\hbar k k_0}{M} \right) b_{g,n} - \frac{i}{2} (V_1 b_{e,n+1} + V_2 b_{e,n-1}), \quad (18)$$

$$\frac{\partial}{\partial t} b_{e,n} = -i \left(n^2 \delta_{\text{rec}} + \frac{n\hbar k k_0}{M} \right) b_{e,n} - \frac{i}{2} (V_1 b_{g,n-1} + V_2 b_{g,n+1}) - \frac{\gamma}{2} b_{e,n}. \quad (19)$$

Here $\delta_{\text{rec}} = \hbar k^2 / (2M)$.

We seek the state vector (11) by the Monte Carlo wave-function method [11,12]. This method, when applied to the

amplitudes of the probabilities $b_{g,n}$ and $b_{e,n}$ to find an atom in the ground or excited states with momentum $\hbar k_0 + n\hbar k$, looks like the following.

(1) We assume that at time t the amplitudes $b_{g,n}(t)$ and $b_{e,n}(t)$ are normalized:

$$\sum_{n=-\infty}^{\infty} [|b_{g,n}(t)|^2 + |b_{e,n}(t)|^2] = 1. \quad (20)$$

Knowing $b_{g,n}(t)$ and $b_{e,n}(t)$, we find the values of $b_{g,n}^{(1)}(t + \Delta t)$ and $b_{e,n}^{(1)}(t + \Delta t)$ from Eqs. (18) and (19) for a small time interval Δt . From the difference

$$1 - \sum_{n=-\infty}^{\infty} (|b_{g,n}^{(1)}(t + \Delta t)|^2 + |b_{e,n}^{(1)}(t + \Delta t)|^2) = \Delta P_{\text{sp}}, \quad (21)$$

we find the probability of an atom to spontaneously emit a photon during the time interval Δt :

$$\Delta P_{\text{sp}} = \gamma \Delta t \sum_{n=-\infty}^{\infty} |b_{e,n}^{(1)}(t)|^2. \quad (22)$$

(2) To find whether there was a photon emission during the time Δt , we generate a random variable, ϵ , which is uniformly distributed between 0 and 1 and compare it with ΔP_{sp} . If $\epsilon > \Delta P_{\text{sp}}$ (in most cases), no emission of a photon has occurred. In this case,

$$b_{g,n}(t + \Delta t) = \frac{b_{g,n}^{(1)}(t + \Delta t)}{\sqrt{1 - \Delta P_{\text{sp}}}}, \quad (23)$$

$$b_{e,n}(t + \Delta t) = \frac{b_{e,n}^{(1)}(t + \Delta t)}{\sqrt{1 - \Delta P_{\text{sp}}}}. \quad (24)$$

If $\epsilon \leq \Delta P_{\text{sp}}$, the atom emits a photon and goes to the ground state. In this case,

$$b_{g,n}(t + \Delta t) = \frac{b_{e,n-\xi}^{(1)}(t + \Delta t)}{\sum_{m=-\infty}^{\infty} |b_{e,m}^{(1)}(t + \Delta t)|^2}, \quad (25)$$

$$b_{e,n}(t + \Delta t) = 0, \quad (26)$$

where ξ takes one of the values $\xi = 0$ and ± 1 with some probability. Here we simulate the real distribution of the projections of the photon momentum on the Oz axis by a hypothetical distribution with $\xi = 0$ and ± 1 , as was done in the modeling of Doppler cooling in Refs. [12,16].

Instead of going back to step 1 and continuing the calculation further, we adjust the numbering of the amplitudes $b_{g,n}(t + \Delta t)$ in order to reduce the required size of the amplitude arrays in numerical calculations. For this purpose, we calculate the average momentum acquired by the atom between the moments of spontaneous photon emission as

$$\langle \Delta p \rangle = \hbar k \sum_{n=-\infty}^{\infty} n |b_{g,n}|^2, \quad (27)$$

and we find the integer number n_{ph} of the photon momentum $\hbar k$ which it contains as follows:

$$n_{\text{ph}} = \left[\frac{\langle \Delta p \rangle}{\hbar k} \right], \quad (28)$$

where square brackets denote an integer part of a number. Next, we change the numbering of the amplitudes:

$$b_{g,n} \rightarrow b_{g,n-n_{\text{ph}}}. \quad (29)$$

This is equivalent to changing the momentum of an atom to $-n_{\text{ph}}\hbar k$, so we also change the momentum,

$$p_0 \rightarrow p_0 + n_{\text{ph}}\hbar k, \quad (30)$$

and return to step 1.

For definiteness, we assume that the atom in the ground and excited states is characterized by angular momentums $\hbar J_g$ and $\hbar J_e$, with $J_e = J_g + 1$. In this case, the two-level scheme of the atom-light interaction between the states $|g, m_g = J_g\rangle$ and $|e, m_e = J_e\rangle$ (these are the states that we denoted for simplicity by $|g\rangle$ and $|e\rangle$) is realized when the atom interacts with circularly polarized light. The optimal description of the momentum diffusion rate due to spontaneous emission by a discrete distribution of the projection of the photon momentum on the axis Oz occurs if ξ acquires the values $-1, 0$, and $+1$ with probabilities of $1/5, 3/5$, and $1/5$ [12,16].

In the calculations, we also use the model of the heavy atom, $M \rightarrow \infty$. In this case, the terms in Eqs. (18) and (19), which contain δ_{rec} , become negligible and these equations read as follows:

$$\frac{\partial}{\partial t} b_{g,n} = -inkv_0 b_{g,n} - \frac{i}{2}(V_1 b_{e,n+1} + V_2 b_{e,n-1}), \quad (31)$$

$$\frac{\partial}{\partial t} b_{e,n} = -inkv_0 b_{e,n} - \frac{i}{2}(V_1 b_{g,n-1} + V_2 b_{g,n+1}) - \frac{\gamma}{2} b_{e,n}, \quad (32)$$

where $v_0 = \hbar k_0/M$ is the initial velocity of the atom. In this approximation, a very small variation of the velocity with time practically does not change the Doppler shift.

IV. NUMERICAL CALCULATION ROUTINE

We consider an ensemble of N atoms in the field of the bichromatic counterpropagating waves and assume that each atom begins to move with a projection v_0 of the initial velocity on the axis Oz . The evolution of the state vector of the atom is calculated by the procedure described in Sec. III. We solve the Schrödinger equation by Runge-Kutta methods of the fourth-order with a time step Δt and every Δt we check the norm of the wave function and use it to decide when a quantum jump is to occur. We repeat this time step many times until we reach the final time of calculation t_f .

Knowing the final state vector of each of the N atoms, we determine the average momentum of the m th atom by the formula

$$\langle p^{(m)} \rangle = p_0^{(m)} + \hbar k \sum_{n=-\infty}^{\infty} n (|b_{g,n}^{(m)}|^2 + |b_{e,n}^{(m)}|^2), \quad (33)$$

where the values of the probability amplitudes refer to the m th atom, and $p_0^{(m)}$ is the initial value of the momentum after the last act of spontaneous radiation, which is modified after each spontaneous photon radiation according to Eq. (30). The average value of the square of the momentum of the m th atom

is calculated by the formula

$$\langle (p^{(m)})^2 \rangle = \sum_{n=-\infty}^{\infty} (p_0^{(m)} + n\hbar k)^2 (|b_{g,n}^{(m)}|^2 + |b_{e,n}^{(m)}|^2). \quad (34)$$

Now we can calculate the average value of the z component of the momentum per an atom in the ensemble,

$$p_{av} = \frac{1}{N} \sum_{m=1}^N \langle p^{(m)} \rangle, \quad (35)$$

and the standard deviation of the z component of the momentum,

$$\Delta p = \sqrt{\frac{1}{N} \sum_{m=1}^N \langle (p^{(m)})^2 \rangle - p_{av}^2}, \quad (36)$$

per an atom from its average value. Equations (35) and (36) allow us to calculate the average force F acting on the atom and the momentum diffusion coefficient D :

$$F = \frac{p_{av}}{t_f}, \quad (37)$$

$$D = \frac{\Delta p^2}{2t_f}. \quad (38)$$

In the following calculations, we compare the force of light pressure on the atom in the field of counterpropagating bichromatic waves with the maximal force F_{rad} of pressure on the atom in the field of the monochromatic traveling wave given by Eq. (1). We compare the momentum diffusion coefficient with the maximal momentum diffusion coefficient D_r in the field of a traveling monochromatic wave along the direction of its propagation [2]:

$$D_r = \frac{1}{4} \hbar^2 k^2 \gamma (1 + \alpha), \quad (39)$$

where $\alpha = \langle \cos^2 \theta \rangle = \frac{2}{5}$ is the mean value of the square of the cosine of the angle between the direction of photon radiation and the direction of wave propagation.

V. RESULTS OF NUMERICAL SIMULATIONS

We perform numerical simulation for the case of sodium atoms. In addition, we consider the limiting case of very heavy atoms, in which the change of the velocity of an atom during the atom-field interaction is negligibly small.

Calculations were carried out for ^{23}Na atoms, in which a cyclic interaction with the field can be created [3]. The wavelength of the transition $3^2S_{1/2} - 3^2P_{3/2}$ in the sodium atom is $\lambda = 589.16$ nm, the rate of spontaneous emission is $\gamma = 2\pi \times 9.795$ MHz, and the Doppler cooling limit is $T_D = 235.03$ μK [17].

A. Sodium atoms in the field of counterpropagating bichromatic waves

Figure 1 shows time evolution of the mean velocity \bar{v} and the standard deviation of the velocity Δv from its mean value for sodium atoms in the field of counterpropagating bichromatic waves. The plots are obtained both for the optimal ratio of $\Omega_R/\delta = \sqrt{6}$ at $\varphi = \pi/4$ [6] and for a small but noticeable

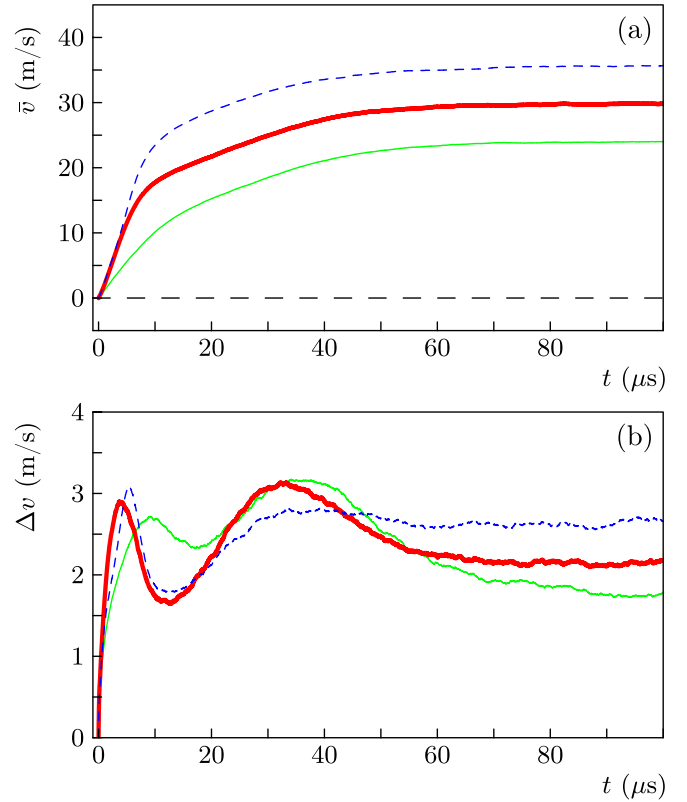


FIG. 1. Time dependence of the average velocity \bar{v} (a) and the standard deviation Δv (b) for 1000 sodium atoms in the field of the counterpropagating bichromatic waves. Parameters are as follows: $\Omega_R = 2\pi \times 122$ MHz, $\delta = 2\pi \times 40$ MHz (thin line), $\delta = 2\pi \times 50$ MHz (thick line), and $\delta = 2\pi \times 60$ MHz (dashed line). The initial velocity of the atoms is $v_0 = 0$. The phase difference of the counterpropagating waves is $\varphi = \pi/4$.

($\approx 20\%$) deviation from the optimum. First of all, it should be noted that with increasing time the velocity of the atom approaches $v = \delta/k$, when, according to the quasiclassical theory [1,5], the force of light pressure exerted on the atom is zero. The standard deviation Δv increases monotonically with time only at the beginning of the interaction of atoms with the field, and then this dependence becomes nonmonotonic. This suggests that the influence of the Doppler effect on the distribution of atoms in the momentum space is significant. In the next section, to exclude the influence of the time-dependent Doppler shift on the light pressure force and the momentum dispersion, we consider the interaction of atoms of very large mass with counterpropagating bichromatic waves.

At the beginning of the interaction of atoms with the field, the dependencies of Δv on t shown in Fig. 1(b) are well approximated by the curves $\Delta v = \sqrt{2D_v t}$, which indicates the diffusion nature of the spreading of the distribution of atoms by momentum with the diffusion coefficient D_v in the velocity space.

The diffusion coefficient D_v is related to the momentum diffusion coefficient D by the formula

$$D_v = D/M^2. \quad (40)$$

Let us compare the diffusion coefficient in the field of counterpropagating bichromatic waves with that in the field of a traveling monochromatic wave of high intensity (when there is a saturation of absorption),

$$D_{vr} = D_r/M^2, \quad (41)$$

where D_r is given by Eq. (39). Calculations for sodium atoms with $\alpha = 0.4$ give $D_r = 2.78 \times 10^{-47} \text{ kg}^2 \text{ m}^2/\text{s}^3$ and $D_{vr} = 19.07 \times 10^3 \text{ m}^2/\text{s}^3$.

For the curves shown in Fig. 1 we have the ratio D_v/D_{vr} : 34.5 ($\delta/2\pi = 40$ MHz), 60.6 ($\delta/2\pi = 50$ MHz), and 47.9 ($\delta/2\pi = 60$ MHz); i.e., the coefficient of momentum diffusion of sodium atoms in the field of counterpropagating bichromatic waves exceeds the coefficient of momentum diffusion in the field of traveling monochromatic wave by 1–2 orders.

There is a well-known analogy between the light pressure force in the field of the counterpropagating bichromatic waves and the sequences of counterpropagating π pulses [1,4–6,10]. We may expect that the momentum diffusion coefficients in these fields are of the same order of magnitude.

The maximal value of the coefficient of diffusion of atoms in the field of counterpropagating sequences of π pulses with the repetition period T for the model of a “heavy” atom in the most interesting case $\gamma T \ll 1$ reaches [10]

$$D_{\pi \max} = \frac{4\hbar^2 k^2}{\gamma T^2}. \quad (42)$$

Substituting $T = \pi/\delta$ in Eq. (42), we obtain a rough estimation of the momentum diffusion coefficient of atoms in the field of the counterpropagating bichromatic waves:

$$D_{\text{bi}} = \frac{4\hbar^2 k^2 \delta^2}{\gamma \pi^2}. \quad (43)$$

For sodium atoms, Eq. (43) gives $D_{\text{bi}} = 8.04 \times 10^{-46} \text{ kg}^2 \text{ m}^2/\text{s}^3$ for $\delta/(2\pi) = 50$ MHz. Estimation of the momentum diffusion coefficient from Fig. 1 for $\delta/(2\pi) = 50$ MHz gives $D = 1.7 \times 10^{-45} \text{ kg}^2 \text{ m}^2/\text{s}^3$, which is twice D_{bi} . We see the close results in the momentum diffusion coefficients calculated from Fig. 1 and from Eq. (43) for the parameters we used.

At the beginning of the interaction of atoms with the field, the standard deviation of the velocity from the mean value changes approximately according to the law $\Delta v \propto \sqrt{2D_v t}$ [see the initial part of Fig. 1(b)]. Over time, the dependence of Δv on time ceases to be monotonic: there are observed areas of growth and the decline of Δv [see Fig. 1(b)]. As far as \bar{v} grows monotonically with time, similar peculiarities are observed for the dependence Δv on \bar{v} [see Fig. 2(b)], which is produced from Figs. 1(a) and 1(b). Figure 2 also shows the dependence of average acceleration a on \bar{v} , which is produced from Fig. 1(a) and $a(t)$. The latter was found by differentiating $\bar{v}(t)$ [Fig. 1(a)] after its presmoothing. Such smoothing is necessary because the time derivative of the unsmoothed \bar{v} has peculiarities due to quantum jumps in the atoms. We approximate the curve by the cubic spline f which minimizes

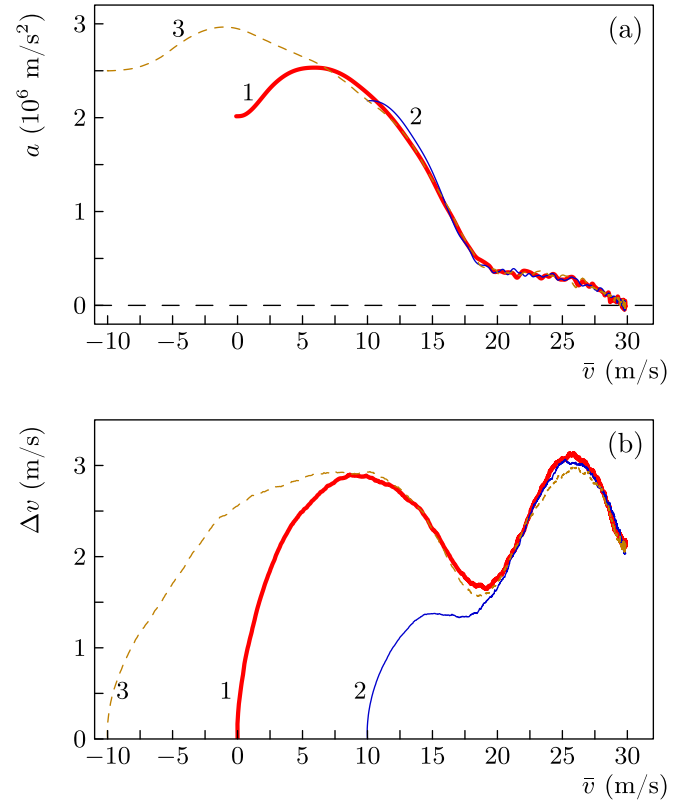


FIG. 2. Correspondence between the average acceleration $a = d\bar{v}/dt$ and the average velocity \bar{v} of atoms (a) and correspondence between the standard deviation of the velocity Δv and \bar{v} of atoms (b) in the field of counterpropagating bichromatic waves. Parameters are as follows: $\Omega_R/(2\pi) = 122$ MHz, $\delta/(2\pi) = 50$ MHz, and $\varphi = \pi/4$. The initial velocity of atoms is $v_0 = 0$ (curve 1), $v_0 = 10$ m/s (curve 2), and $v_0 = -10$ m/s. Simulation is for 1000 sodium atoms. The time of the atom-field interaction is 100 μs .

the functional

$$J[f] = w \sum_{j=1}^K [f(x_j) - y_j]^2 + \int_{x_1}^{x_K} [f'(x)]^2 dx. \quad (44)$$

Here x_j and y_j are the coordinates of the j point of the curve, K is the number of points, and w is the point's weight. When w approaches 0, the second term dominates and the spline approaches a straight line. In the opposite case of very large w , the spline almost passes the data points. We used $w = 1.0$ for $K = 4001$ points. The commands which produce the smoothed curve when using GNU PLOT software are

```
set samples 4001
plot [:][:] 'data' using 1:2:(1.0) with lines
smooth acsplines
```

The same result may be obtained by function `csaps(x,y,q,x,w)` of MATLAB or OCTAVE with weight $w = 1.0$ and $q = 0.5$.

To understand the nonmonotonic change of Δv with a change of \bar{v} , we must take into account two factors that determine it. On the one hand, it is a process of momentum diffusion, which leads to a diffusionlike change of Δv with time. On the other hand, the dependence of the average acceleration a on the average velocity \bar{v} of an atom can both

increase and decrease the value of Δv . Indeed, let us consider the case $da/d\bar{v} < 0$. It is plausible to assume that the acceleration a_1 of one atom or group of atoms with velocity v_1 also decreases with increasing velocity, $da_1/dv_1 < 0$. The accuracy of this statement becomes greater if the standard deviation Δv of the velocity of atoms in the ensemble from its mean value becomes smaller. In this case, the acceleration of atoms with a lower velocity is greater than the acceleration of atoms with a higher velocity. As a result, the velocity distribution of atoms narrows to a limit that is established as a result of the dynamic equilibrium of the distribution narrowing process by reducing the acceleration of atoms with increasing velocity and the momentum diffusion process that makes this distribution broader. A well-known analog of this phenomenon is the Doppler cooling of atoms [8], with the difference that instead of grouping atoms at zero velocity in the field of a standing monochromatic wave, we have the grouping of atoms near the average velocity of the ensemble of atoms \bar{v} in the field of counterpropagating bichromatic waves in the case of $da/d\bar{v} < 0$. Similar considerations show that in the case of $da/d\bar{v} > 0$ there should be an expansion of the distribution of atoms by momentum. Besides that, in this case, the dependence of the acceleration of atoms on their velocity changes Δv in the same direction as the momentum diffusion.

The reason for the shift of the first maximum of the dependence $\Delta v(\bar{v})$ relative to the first maximum of $a(\bar{v})$ towards the larger \bar{v} in Fig. 2 is obvious: the derivative $da/d\bar{v}$ near the maximum of the dependence $a(\bar{v})$ is too small to compensate for the increase in Δv due to the momentum diffusion. The small value of the derivative $da/d\bar{v}$ in the range from 20 to 25 m/s, which is insufficient to compensate for the momentum diffusion, is the reason for the growth of Δv in Fig. 2(b).

In Fig. 2 we see that the final average velocities of groups of atoms that start with initial velocities $v_0 = -10$ m/s, $v_0 = 0$ m/s, and $v_0 = 10$ m/s after $100 \mu\text{s}$ are close to $\delta/k = 29.46$ m/s for which the light pressure force is close to zero [1]. At the same time Δv almost coincides for these groups of atoms and is approximately equal to 2.1 m/s. This means that the bichromatic force cools atoms: atoms with initial velocities from -10 to 10 m/s after $100 \mu\text{s}$ of interaction with the bichromatic waves are characterized by $\Delta v \sim 2$ m/s. The simulation also shows that the atoms with $v_0 = 20$ m/s finish with \bar{v} close to δ/k and Δv close to 2 m/s, but when we enlarge the initial velocity in the negative direction the result is worse. For $v_0 = -25$ m/s, the final \bar{v} is close to δ/k , but $\Delta v = 7.18$ m/s.

Since the velocity of atoms changes continuously with time, the momentum diffusion coefficient also changes with time. To completely exclude the effect of a change in velocity on the momentum diffusion coefficient, in the next section we consider the model of the “heavy atom,” in which the change of atomic velocity is small enough to neglect changes of Doppler shift. In addition, this consideration allows us to compare the results of the calculation of the light pressure force exerted on an atom in the quasiclassical theory [1,6,7] with the results of the quantum mechanical theory. Since the quasiclassical theory considers an atom as a material point, and in our calculations, the wave function of an atom at the initial time is an eigenstate of the momentum, consistency

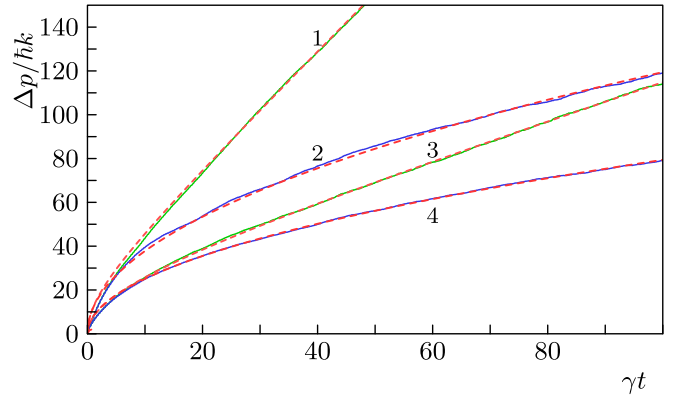


FIG. 3. Time dependence of the standard deviation Δp of the atom's momentum from its average value for 1000 atoms and $\Omega_R = 24.5\gamma$ and $\delta = 10\gamma$. Parameters are as follows: curve 1, $kv = 0$; curve 2, $kv = 0.2\gamma$; curve 3, $kv = 5\gamma$, and curve 4, $kv = 5.05\gamma$. Phase difference of the counterpropagating waves is $\varphi = \pi/4$. Solid lines are the results of numerical calculations, and dashed lines are approximation of curves 1 and 3 by formulas $\Delta p = \sqrt{2Dt + St^2}$ (curves 1 and 3) and $\Delta p = \sqrt{2Dt}$ (curves 2 and 4). The approximation parameters are as follows: $D = 69.92\hbar^2 k^2 \gamma$, $S = 6.88\hbar^2 k^2 \gamma^2$ (curve 1), $D = 71.35\hbar^2 k^2 \gamma$ (curve 2), $D = 59.51\hbar^2 k^2 \gamma$ and $S = 0.729\hbar^2 k^2 \gamma^2$ (curve 3), and $D = 31.52\hbar^2 k^2 \gamma$ (curve 4).

of the results obtained from these different assumptions are important for the confident application of the quasiclassical approach to the light pressure force calculation.

B. Heavy atoms in the field of counterpropagating bichromatic waves

We simulate the motion of “heavy” atoms in the field of the counterpropagating waves by the procedure described in Sec. IV and we use Eqs. (31) and (32), which give the time evolution of the probability amplitudes $b_{g,n}$ and $b_{e,n}$. Calculating the change of the average momentum of the atoms during the time $\sim 100\gamma^{-1}$, much greater than the time of the transient processes at the beginning of the interaction of atoms with the field ($\sim 10\gamma^{-1}$), we find the average force exerted on an atom. In addition, we calculate the light pressure force by the density matrix method according to the theoretical work [1] to verify the correctness of our software.

First of all we simulated the time dependence of Δp for different ratios δ/Ω_R and found that this dependence dramatically changes with δ/γ starting from the momentum diffusion law $\Delta p \sim \sqrt{t}$ ($\delta = 0$, i.e., standing wave) to practically linear dependence, $\Delta p \sim t$ ($\delta \sim \Omega_R$). The latter case contradicts the diffusionlike dependence $\Delta v(t)$ shown in Fig. 1(b). As far as the dependencies depicted in Fig. 1 are calculated taking into account the change in the velocity of atoms over time, we also investigate the dependence $\Delta p(t)$ for a nonzero initial velocity of a “heavy” atom.

Figure 3 shows an example of the time dependence of the standard deviation Δp of the atom's momentum from its average value for $\Omega_R = 24.5\gamma$ and $\delta = 10\gamma$ ($\Omega_R \approx \sqrt{6}\delta$). In two cases the dependence of $\Delta p(t)$ is linear for $\gamma t > 10$ (curve 1) and $\gamma t > 20$ (curve 3). In the other two cases, if the ratio kv/γ is not very

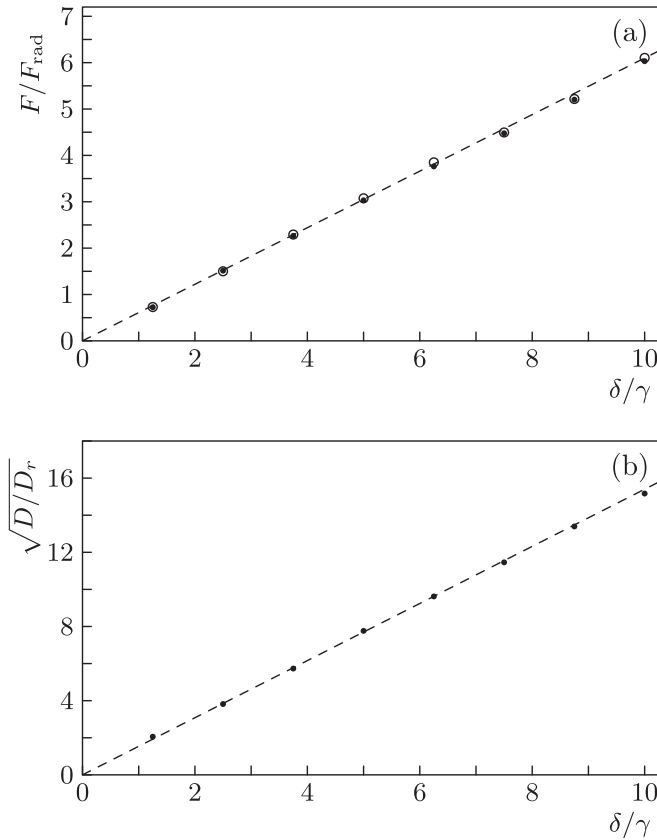


FIG. 4. The dependence of the light pressure force exerted on atoms in units of F_{rad} (a) and the square root of the coefficient of momentum diffusion \sqrt{D} in units of $\sqrt{D_r}$ (b) on δ/γ provided that $\Omega_R = \sqrt{6}\delta$ and $\varphi = \pi/4$. Averaging is per 1000 atoms. Open circles correspond to $v = 0$, and solid circles correspond to $kv = 0.1\gamma$.

small, the dependence of $\Delta p(t)$ can be approximated by $\Delta p = \sqrt{2Dt}$ (see dashed lines). The initial parts of the curves, $\gamma t < 1$, are almost linear. This is the expected result: there is no momentum diffusion before spontaneous emission occurs. Here the momentum distribution becomes wider due to the scattering of atoms by the counterpropagating bichromatic waves. The scattering parts are also observed on curves 1 and 3 in the region $\gamma t \gg 1$; in these cases, the scattering occurs due to Doppleron resonances [18,19] and the time dependence of Δp is approximately described by the formula

$$\Delta p = \sqrt{2Dt + St^2} \quad (45)$$

(see dashed lines for curves 1 and 3 in Fig. 3). Equation (45) manifests the time dependence of $(\Delta p)^2$ as a sum of two terms, $2Dt$ and St^2 , one which describes the momentum diffusion of atoms, while the other is responsible for scattering.

The scatteringlike time dependence of Δp at the resonance (curve 3) changes to a diffusionlike one (curve 4) even if the detuning from the resonance is very small (1%). At the resonance we characterize $\Delta p(t)$ by two constants, D and S , while otherwise only one constant, D , is sufficient.

At the end of the discussion of Fig. 3, we note small oscillations with the period π/kv on curve 2. These oscillations

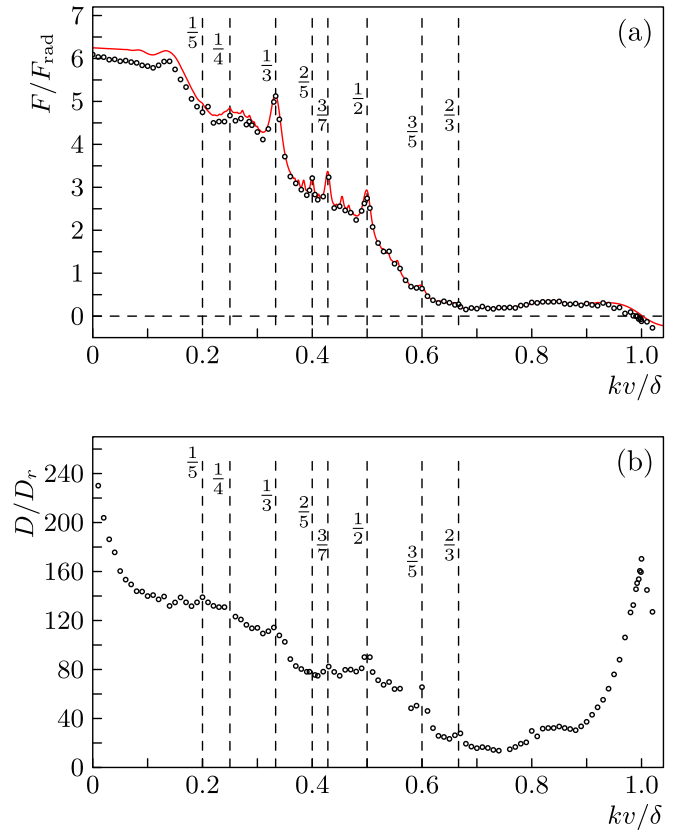


FIG. 5. The dependencies of the light pressure force F exerted on atoms in units of F_{rad} (a) and the momentum diffusion coefficient D in units of D_r (b) on the atomic velocity for $\Omega_R = \sqrt{6}\delta$, $\delta = 10\gamma$, and $\varphi = \pi/4$. Averaging is per 1000 atoms. Circles show the results of calculation by the Monte Carlo wave-function method, and the solid curve is the result of calculations by the density matrix equation. Dashed vertical lines mark the values of kv/δ , which correspond to Doppleron resonances. The momentum diffusion coefficients for these values of kv/δ are not defined.

are more prominent on the dependence $\Delta p(t)$ for $kv = 0.1\gamma$, not shown here.

Figure 4 shows the dependence of the light pressure force and the square root of the momentum diffusion coefficient on δ provided that the optimal conditions $\Omega_R = \sqrt{6}\delta$ and $\varphi = \pi/4$ of the atom-field interaction are met. Using the dependence shown in Fig. 4(b), we find the following for the parameters of Fig. 4:

$$D \approx 2.4D_r \frac{\delta^2}{\gamma^2}. \quad (46)$$

This is about twice as much as given by Eq. (43).

As far as both F and \sqrt{D} under optimal conditions linearly depend on δ , $\Delta p/\bar{p} = \sqrt{2Dt}/(Ft) \approx 4.2/\sqrt{\gamma t}$ does not depend on δ . Since $\Omega_R = \sqrt{6}\delta$, the momentum diffusion coefficient under optimal conditions is proportional to Ω_R^2 , i.e., the intensity of the laser radiation.

Figure 5 shows an example of the dependence of the light pressure force exerted on atoms and the momentum diffusion coefficient for the optimal parameters of the atom-field interaction, which were found from the evolution of the atom's momentum distribution during time $t = 100/\gamma$. Besides that,

the result of the light pressure force calculation by the equations for the density matrix [1,5] is also presented. Some differences in the calculation by both methods can be explained by the different descriptions of the atom: in this paper, an atom is described by a wave packet; in Refs. [1,5] an atom is a material point. The momentum diffusion coefficient at velocities corresponding to Doppleron resonances could not be calculated because the time dependence of the momentum variance does not obey the law $\Delta p^2 = 2Dt$. It is noteworthy that the coefficient of momentum diffusion with increasing velocity v of atoms at $kv < 0.05\gamma$ decreases rather quickly, almost twice that when velocity changes from $v = 0.01\delta/k$ to $v = 0.1\delta/k$, while the light pressure force remains almost unchanged in this velocity range.

VI. CONCLUSIONS

We showed that the standard deviation of the velocity from its average value may increase or decrease with time. There are two factors that control these phenomena. One of them is the momentum diffusion of atoms, which always spreads the momentum distribution. The other has a dynamic nature. If the acceleration of atoms increases when their velocity increases, the broadening of the velocity distribution of the atomic ensemble takes place. In the opposite case, the bunching of atoms around the average velocity of the atomic ensemble occurs.

To separate the influence of momentum diffusion on the evolution of momentum distribution of atoms from the influence of the time-dependent Doppler shift of the atomic frequency, we used the model a “heavy” atom, in which the change of the Doppler shift during the interaction of an atom with the field can be neglected. In the frame of this approximation, we find that the time dependence of Δp in the vicinity of Doppleron resonances becomes almost linear if the time of the atom-field interaction is large enough. In other cases, $\Delta p(t)$ is described by the diffusion law.

The estimation of the momentum diffusion coefficient based on the results of numerical simulation of the velocity evolution of Na atoms in the field of the counterpropagating bichromatic waves roughly agrees with its estimation according to the formula for the maximum diffusion coefficient of atoms in the field of the counterpropagating sequences of π pulses.

For optimal parameters of the atom-field interaction, the coefficient of momentum diffusion is proportional to the intensity of laser radiation.

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