

# Particle selection by a gradient force in a laser near field

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It is shown that the spatial inhomogeneity of the intensity distribution of laser radiation diffracted by an opening that is small in comparison with the wavelength leads to resonant selection of atoms due to the resulting gradient dipole force acting on the atom. As a result, the flux of atoms passing through the opening increases or decreases, depending on the frequency offset of the laser field relative to the frequency of the atomic transition. This effect is sensitive to the type of atom, its velocity, and its direction as it passes through the opening.

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## 1. INTRODUCTION

The advent of lasers and the invention of a number of methods of selective action of laser radiation on atoms and molecules have opened up new possibilities in the selection of atoms and molecules, and in particular, isotopes (see Ref. 1). However, the most effective laser methods are destructive since they are based on the photoionization of atoms and photodissociation of molecules. It is of fundamental interest to search for other methods of selection, even without regard to their practical application. Methods of this kind include those based on resonant action of light on atoms.<sup>2,3</sup>

The possibility of using a spontaneous resonance force to select atomic isotopes was considered in Refs. 4 and 5. In the present paper, an extension of Ref. 6, we propose a non-destructive way of sorting neutral, slow (cold) atoms and molecules, based on the use of the dipole gradient force that arises in the near field of resonant laser light diffracted by a circular opening small in comparison with the wavelength.

The structure of this near field is most remarkable and was analyzed in detail in Refs. 7 and 8 (see also Ref. 9), in which relatively simple analytic expressions were found for the fields. The same notation will be used here as in those papers.

By the right choice of frequency and intensity of the laser light, it is possible to vary the magnitude of the atomic flux through an opening and to bring about preferential passage through the opening of one or another sort of particle, which ultimately leads to particle selection. The geometry of the problem is shown in Fig. 1. It is not our goal to create an industrial method of isotope selection. Rather, the idea here is to design a more sensitive scientific instrument intended, for example, for the selection of enantiomers, and also a check the fundamental relations between information and entropy.<sup>10</sup>

In Sec. 2 we examine the variation in particle flux through a small opening when this opening is illuminated by resonant laser light, for which we introduce the concept of the effective cross section of the opening. We then find analytic expressions for the effective cross section within the framework of perturbation theory, which we compare with

the results of computer modeling. In Sec. 3 we present analytic expressions for the effective cross section when a quasiequilibrium gas is made to flow through a small opening irradiated by resonant laser radiation. In Sec. 4 the results of Secs. 2 and 3 are illustrated by selecting <sup>20</sup>Ne and <sup>22</sup>Ne isotopes using the <sup>1</sup>S<sub>5</sub>→<sup>2</sup>P<sub>9</sub> transition. We conclude by analyzing the results and indicating directions for future work.

## 2. SELECTION OF AN ATOMIC BEAM NORMALLY INCIDENT ON AN ILLUMINATED OPENING

The essence of the effect considered here is illustrated in Figs. 1(a) and 1(b), in which the solid curves represent the energy density contours of laser light with a negative frequency offset, diffracted by a small-diameter opening (diameter  $2a$ , where  $a \ll \lambda$ ). The gradient of the energy density determines the magnitude of the force on the atom.<sup>11</sup> Figure 2 shows the dependence of the mean square of the electric field in the vicinity of the opening. The magnitude of the gradient force depends not only on the intensity gradient, but also on the magnitude and sign of the laser frequency ( $\omega$ ) offset relative to the resonance point  $\omega_0$  of the atomic transition (see Ref. 12).

If the laser frequency  $\omega$  has a negative offset  $\Omega = \omega - \omega_0 < 0$ , the gradient force pulls the selected atoms into the stronger field region, so that the particle flux through the opening grows in comparison with the case of no near field. A positive offset produces the opposite result.

It is convenient to describe the flux variation by introducing an effective particle capture cross section for the opening plus field,  $S_{\text{eff}} = \pi r_{\text{eff}}^2$ , so that the flux variation is described by  $S_{\text{eff}}/S_0 = r_{\text{eff}}^2/a^2$ .

Strictly speaking, two cases of interaction of the atoms with the near field are possible: 1) motion of the atoms into the oncoming field, in which an atom begins to interact with the field while in the ground state (the “dressed” state) (Ref. 13) and remains in it for a short interaction time (Fig. 1a, and 2) motion of atoms in the same direction as the incident laser light, in which an atom begins to interact with the diffracted field while in a mixed state (Fig. 1b) due to a lengthy inter-

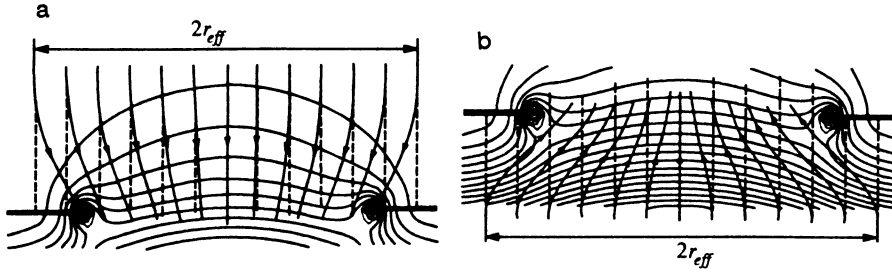


FIG. 1. Geometry of the problem in the case of an attractive gradient force for motion of the atoms counter to the incident light wave (a) and in the same direction with it (b). The dashed lines correspond to the trajectories of the atoms without the laser field. The solid lines with arrows correspond to the trajectories of the atoms in the presence of the field. The solid lines without arrows are level lines of the potential of the gradient force.

action with the field of the standing wave formed in front of the obstacle.

In the first case, the potential of the gradient force is given by<sup>13</sup>

$$U = \frac{\hbar\Omega}{2} \left( \sqrt{1 + 2 \frac{\mu^2 \langle E^2 \rangle}{\hbar^2 |\gamma|^2}} - 1 \right), \quad (1)$$

and in the second, by<sup>14</sup>

$$U = \frac{\hbar\Omega}{2} \ln \left( 1 + \frac{\mu^2 \langle E^2 \rangle}{\hbar^2 |\gamma|^2} \right). \quad (2)$$

Here  $\mu$  is the electric dipole moment of the transition,  $|\gamma|^2 = \Omega^2 + (\Gamma/2)^2$ ,  $\Omega = -\omega_0$ ,  $\omega$  and  $\omega_0$  are the laser frequency and the transition frequency, respectively, and  $\Gamma$  is the total width of the transition.  $\langle E^2 \rangle$  is the mean square of the electric field, which in the case of normal incidence of a circularly polarized wave

$$\mathbf{E}_{\text{in}} = \frac{E_{0m}}{\sqrt{2}} (\cos(\omega t - kz), \sin(\omega t - kz), 0), \quad (3)$$

$$\mathbf{H}_{\text{in}} = \frac{E_{0m}}{\sqrt{2}} (-\sin(\omega t - kz), \cos(\omega t - kz), 0),$$

is given by<sup>7,8</sup>

$$E^2 = \left( \frac{kaE_{0m}}{3\pi} \right)^2 \mathcal{E}(r, z),$$

where

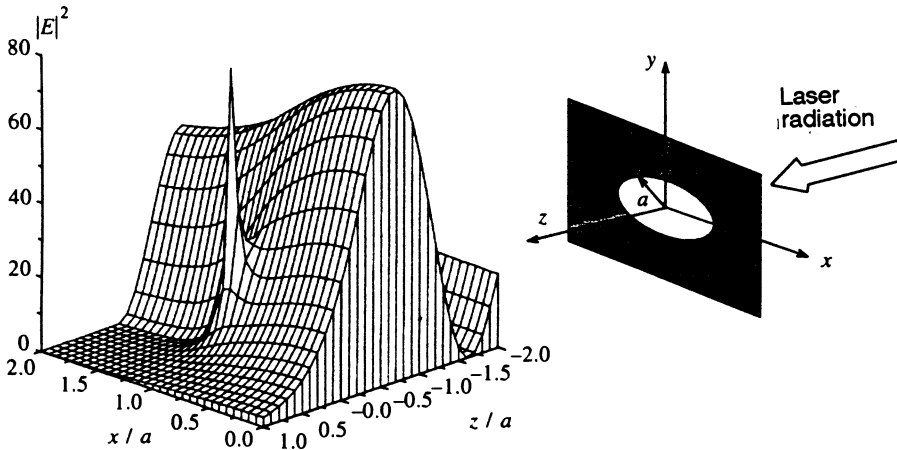


FIG. 2. Three-dimensional distribution of the mean square of the electric field of the laser radiation in the vicinity of the opening ( $ka=2$ ,  $E_{0m}=3\pi/2$  CGS units).

$$\mathcal{E} = \begin{cases} 18\pi^2 \frac{\sin^2(kz)}{(ka)^2} - 6\pi \frac{\sin(kz)}{ka} \\ \times (2A+B) + A^2 + (A+B)^2 + C^2, & z < 0 \\ A^2 + (A+B)^2 + C^2, & z > 0 \end{cases} \quad (4)$$

where

$$A = R^- \left( \frac{2a^2}{R^*} + 2 - \frac{z^2}{r^2} \right) + za \left( \frac{R^+}{r^2} - \frac{3}{a^2} \arctan \frac{1}{R^+} \right)$$

$$B = R^- \left( \frac{2z^2}{r^2} - \frac{2r^2 - z^2}{R^*} \right) + azR^+ \left( \frac{1}{R^*} - \frac{2}{r^2} \right)$$

$$+ \frac{3zr^2R^+}{aR^*(1+R^{+2})}, \quad C = \frac{2arR^+}{R^*(1+R^{+2})},$$

$$R^* = \sqrt{(R^2 - a^2)^2 + 4a^2z^2}, \quad R^\pm = \sqrt{\frac{R^* \pm (R^2 - a^2)}{2a^2}},$$

$$R^2 = r^2 + z^2. \quad (5)$$

In the case of normal incidence the problem becomes planar, and the motion of an atom in potential (1) or (2) is given by Newton's laws,

$$M\ddot{x} = -\frac{\partial U}{\partial x}, \quad M\ddot{z} = -\frac{\partial U}{\partial z} \quad (6)$$

or Hamilton's equations,

$$M\dot{x} = p, \quad \dot{p} = -\frac{\partial U}{\partial x}, \quad M\dot{z} = q, \quad \dot{q} = -\frac{\partial U}{\partial z}. \quad (7)$$

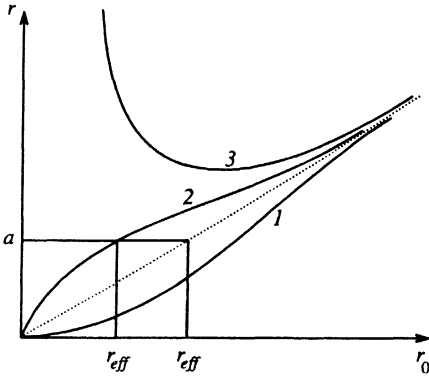


FIG. 3. Qualitative dependence of the radius of the point of impact on the screen,  $r$ , on the impact parameter  $r_0$  in the case of an attractive (1) and a repulsive (2,3) potential.

For definiteness we assume throughout that motion takes place in the  $xz$  plane;  $M$  is the mass of the particles.

The nature of the motion of an atom depends critically on the sign of the frequency offset of the laser illumination, since the gradient force can be either attractive or repulsive. Repulsion is simpler, since trajectories up to the screen do not change substantially in comparison with the no-potential case. In attraction, a particle approaches the screen monotonically (along the  $z$  axis). For radial motion there is a potential well, in the vicinity of the opening so it can in principle be oscillatory. Thus, if we plot the qualitative dependence of the radius  $r$  (from the center) of the point of impact of the particle on the screen on the impact parameter  $r_0$  of the particle, then for a negative offset (an attractive potential) it will look like Fig. 3 (curve 1). Interestingly enough, at low enough velocities, the atom can fly through the opening and then fly back out. Figure 4a shows such trajectories. We, however, will not take effects of this kind into account in our study of the effective cross section, both because of their small effect and the need for special measures to collect the atoms that have passed through.

In the case of positive offsets (repulsive potential), the particle trajectories are more complicated. Some of them (curve 3), in spite of repulsion, go through the opening, some collide with the screen, and some, for a large enough potential gradient, are completely reflected (curve 2). Moreover, if

the particle velocity of the beam is not high enough, total reflection of the entire beam is possible. Such trajectories are shown in Fig. 4b. Figure 3 (curve 2) shows the qualitative dependence of the radius of impact of the particle as a function of its impact parameter.

In either case, determining the effective capture radius of the beam particles reduces to solving the equation

$$r(r_{\text{eff}}, z=0) = a \quad (8)$$

that is, of course, if it exists. Here  $r=r(r_0, z)$  is the equation of the particle trajectory. Before solving Eq. (8), we must first find the trajectory of the atom by solving Newton's equations (6) and (7). Here, depending on the parameters of the problem, various approaches are possible.

Thus, if the velocities of the particles are high enough, the potential can be considered a perturbation, and can serve as the basis of a proper perturbation theory. If, however, the potential cannot be considered a perturbation, we must use numerical methods.

To start with, we consider a small potential. To construct the perturbation theory, we assume that

$$h^* = \frac{4G}{1+\Delta^2} \ll 1, \quad \varepsilon = \frac{\hbar\Gamma}{4T_0} \frac{G\Delta}{1+\Delta^2} \left( \frac{ka}{3\pi} \right)^2 \ll 1. \quad (9)$$

Here  $G$  is the saturation parameter of the transition in the incident field (without the screen),  $\Delta=2\Omega/\Gamma$ , and  $T_0$  is the kinetic energy of the atoms. These conditions can easily be satisfied. Thus, for example, for a beam of neon atoms ( $^1s_5 \rightarrow ^2p_9$  transition) with velocity 1 m/s, the most important parameter  $\eta = \hbar\Gamma/2T_0 \approx 0.16$  is already small, and by an appropriate choice of offset we can always satisfy (9).

If the first of these two conditions is satisfied, the square root in Eq. (1) and the logarithm in Eq. (2) can be expanded in Taylor series, whereupon expressions (1) and (2) both reduce to

$$U = \frac{\hbar\Gamma\Delta}{1+\Delta^2} \left( \frac{\mu}{\hbar} \right)^2 \langle E^2 \rangle \ll T_0. \quad (10)$$

WE now find the effective cross section of the opening as given by perturbation theory. To start with, we consider the simpler case in which the particle and laser beams propagate in opposite directions (Fig. 1a). In this case, prior to the

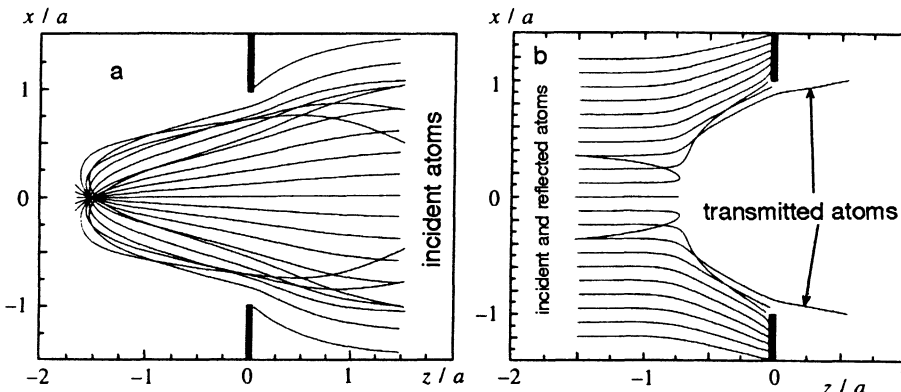


FIG. 4. Trajectories of  $\text{Ne}^{20}$  atoms with turning points beyond the opening in the case of (a) an attractive potential (the beam propagates counter to the radiation,  $\Delta = -1000$ ,  $G = 10^6$ ,  $ka = 2$ ,  $V_0 = 3$  m/s), and (b) a repulsive potential (the beam propagates in the same direction as the radiation,  $\Delta = 1000$ ,  $G = 10^6$ ,  $ka = 2$ ,  $V_0 = 12.85$  m/s).

interaction with the screen, the beam particles do not interact with the standing wave formed by reflection of the incident laser radiation from the screen.

In the zeroth approximation, the influence of the gradient force can be neglected, and the motion of the atoms is given by

$$z^{(0)} = -V_0 t, \quad x^{(0)} = x_0, \quad (11)$$

where  $x_0$  is the impact parameter of the trajectory and  $V_0$  is the initial velocity of the atom. The first-order corrections to these equations are given by

$$M\ddot{x}^{(1)} = -\frac{\partial U}{\partial x}(x=x^{(0)}, z=z^{(0)}), \quad (12)$$

$$M\ddot{z}^{(1)} = -\frac{\partial U}{\partial z}(x=x^{(0)}, z=z^{(0)}),$$

the solutions of which can be found by quadratures:

$$Mx^{(1)} = -\frac{\partial}{\partial x_0} \int_{-\infty}^t U(x_0, -V_0 t')(t-t') dt', \quad (13)$$

$$Mz^{(1)} = -\int_{-\infty}^t \frac{\partial}{\partial z^{(0)}} U(x_0, z^{(0)}(t'))(t-t') dt'.$$

Obviously, the time of impact with the screen differs only slightly from zero, so that we can expand (13) in powers of the dimensionless time  $\tau = V_0 t/a$ . As a result, the equations of motion in  $x$  and  $z$  (dimensionless coordinates  $\tilde{x} = x/a$ ;  $\tilde{z} = z/a$ ) take the form

$$\begin{aligned} \tilde{x} = \tilde{x}_0 - \varepsilon \frac{\partial}{\partial \tilde{x}_0} \left[ \int_0^\infty \tilde{z}' \mathcal{E}(\tilde{x}_0, \tilde{z}') d\tilde{z}' + \tau \int_0^\infty \mathcal{E}(\tilde{x}_0, \tilde{z}') d\tilde{z}' \right. \\ \left. + O(\tau^2) \right], \end{aligned} \quad (14)$$

$$\tilde{z} = -\tau + \varepsilon \int_0^\infty \mathcal{E}(\tilde{x}_0, \tilde{z}') d\tilde{z}' + \varepsilon \tau \mathcal{E}(\tilde{x}_0, 0) + O(\varepsilon \tau^2).$$

The small dimensionless parameter  $\varepsilon$  and the dimensionless square of the electric field  $\mathcal{E}$  have already been introduced [see Eqs. (9) and (4)].

Now, eliminating time from these equations with the help of the equation  $z=0$ , and retaining terms up to first order in  $\varepsilon$ , we obtain an equation relating the radius  $x$  (or  $r$ ) of the point of impact of the atom with the screen to the impact parameter  $x_0$  (or  $r_0$ ):

$$\tilde{x} = \tilde{x}_0 - \varepsilon \frac{\partial}{\partial \tilde{x}_0} \int_0^\infty \tilde{z}' \mathcal{E}(\tilde{x}_0, \tilde{z}') d\tilde{z}'. \quad (15)$$

Now, setting  $x$  equal to  $a$  and solving the resulting equation to first order in  $\varepsilon$ , we obtain the final expression of the effective radius  $r_{\text{eff}}$  of the opening when the atomic beam and the laser beam propagate in opposite directions:

$$r_{\text{eff}} = a \left( 1 + \varepsilon \int_0^\infty \tilde{z}' \frac{\partial \mathcal{E}}{\partial \tilde{x}}(\tilde{x}, \tilde{z}') d\tilde{z}' \right)_{\tilde{x}=1}. \quad (16)$$

The integral in this expression is a universal constant; having computed it, we finally obtain

$$r_{\text{eff}} = (1 - 5.21\varepsilon)a. \quad (17)$$

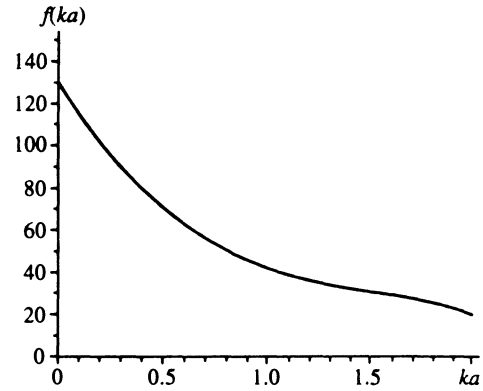


FIG. 5. The function  $f(ka)$ .

As can be seen from (9), for a negative offset  $\varepsilon < 0$ , the effective cross section is greater than when there is no laser illumination, and conversely for a positive offset.

We now consider an atomic beam and laser beam that propagate in the same direction (Fig. 1b). In this case, we can perform completely analogous calculations, as a result of which we obtain the following expression for the effective radius of the opening:

$$r_{\text{eff}} = a \left( 1 - \varepsilon \int_{-\infty}^0 \tilde{z}' \frac{\partial \mathcal{E}}{\partial \tilde{x}}(\tilde{x}, \tilde{z}') d\tilde{z}' \right)_{\tilde{x}=1}. \quad (18)$$

An important difference between (18) and (16) is that the integral in (18) is now a universal function of  $ka$ , and not a universal constant as in (16):

$$r_{\text{eff}} = a[1 - \varepsilon f(ka)]. \quad (19)$$

A graph of this function is shown in Fig. 5. For small  $ka$  ( $0 < ka < 2$ ), it is possible to find a good polynomial approximation to this function:

$$\begin{aligned} f(x) = a_0 + x\{a_1 + x[a_2 + x(a_3 + a_4x)]\}, \\ a_0 = 129.55, \quad a_1 = -158.839, \quad a_2 = 87, \\ a_3 = -14.06, \quad a_4 = -1.67. \end{aligned} \quad (20)$$

The dependence of the effective cross section  $s_{\text{eff}}$  on the relative frequency offset  $\Delta$  is shown by the dashed curve in Figs. 6a and 6b.

Expression (17) and (19) for the effective cross section of the opening, found within the framework of perturbation theory, have a large, albeit bounded, region of applicability, and where conditions (9) are not satisfied to a sufficient degree it is necessary to use numerical methods.

In an attractive potential gradient, the topology of the trajectory up to the plane of the screen is simple (it has no turning points), and after eliminating time and invoking energy conservation, Hamilton's equation (7) reduce to a system of two first-order differential equations,

$$x' = \frac{p}{q(x, z, p)}, \quad p' = \frac{\partial}{\partial x} q(x, z, p), \quad (21)$$

where

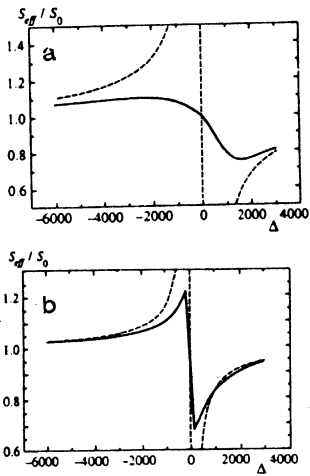


FIG. 6. Relative effective capture cross section of  $\text{Ne}^{20}$  atoms as a function of the relative frequency offset  $\Delta$  of the field in units of  $\Gamma/2$  for  $G=10^6$ ,  $ka=2$ ,  $V_0=15$  m/s. The solid line plots the result of numerical modeling, and the dashed line plots the approximate analytic solution obtained by perturbation theory: a) atoms move in the same direction as the field; b) atoms move counter to the field.

$$q(x, z, p) = \pm \sqrt{2M(T_0 - U) - p^2},$$

and a prime denotes a derivative with respect to  $z$ , while the sign of the square root is determined by the direction of propagation of the beam.

Supplying system (21) now with boundary conditions

$$p(z = \pm\infty) = 0 \quad (\text{normal incidence}),$$

$$x(z=0) = a \quad (\text{trajectory incident at the boundary of the opening}),$$

we have a well-posed boundary-value problem, which can be solved to yield  $x(\infty) = r_{\text{eff}}$ .

To solve this boundary problem, we apply the shooting method,<sup>15</sup> where the test shot proceeds in two steps: first by dichotomy and then by the secant method. The shot itself is realized by solving (21) with initial conditions  $p(\pm\infty) = 0$ ,  $x(\infty) = x_0$ , where  $x_0$  is some value of the impact parameter, generally different for each shot. The trajectory of the particle is determined by integrating (21) using the Runge–Kutta–Feldberg method of order 4–5.<sup>16</sup>

For a positive frequency offset, especially with sufficiently slow atoms, turning points of the trajectories are possible, and even total reflection. Because of the highly varied character of the trajectories (see Fig. 4b), determining the effective cross section with the method described above (for a negative frequency offset) is more difficult, and for a positive offset the effective capture cross section was determined by direct modeling of the beam particle trajectories, with subsequent selection of those particles that passed through the opening. The particle trajectories in this case were also calculated with the help of the Runge–Kutta–Feldberg method of order 4–5.<sup>16</sup>

The results obtained with the help of perturbation theory and numerical modeling of the passage of a beam of  $\text{Ne}^{20}$  atoms with a velocity of 15 m/s through an opening illuminated by laser light are shown in Figs. 6a and 6b for various values of the relative frequency offset and  $G=10^6$ . Analysis of these figures shows, first of all, that laser illumination of a

small opening has a substantial effect on the flux of atoms passing through it; second, the effect substantially depends on the direction of propagation of the atomic beam relative to the laser field; third, the results obtained via perturbation theory have a broad range of applicability (especially for counterpropagating beam and radiation). The agreement improves as the velocities increase.

Thus, a laser near field is capable of having an efficient influence on sufficiently cold and slow atomic and molecular beams. For a more accurate determination of the effective scattering cross section, it is necessary to take into account small corrections associated with the atoms' turning back after passing through the opening. For faster atoms it is necessary to use more accurate expressions for the gradient force that depend on velocity.<sup>13</sup>

### 3. INFLUENCE OF THE NEAR FIELD ON THE RATE OF OUTFLOW OF AN EQUILIBRIUM GAS THROUGH A CIRCULAR OPENING

The results of the preceding section demonstrate that laser illumination of the opening has a substantial effect on the rate of passage through it of a single-velocity beam of neutral particles. In connection with this, it is of interest to investigate the effect that illuminating the opening has on the rate of outflow of a gas of neutral particles whose velocity distribution is not single-velocity, but, say, Maxwellian.

Note that in the absence of laser light, the rate of outflow of particles of one kind or another from the opening depends on their thermal velocity or (in equilibrium) on their mass. In our case, a dipole gradient force exerts a much greater influence, and therefore the velocity effect will not be mentioned again in what follows.

If we assume that after turning on the laser illumination enough time has passed for the establishment of equilibrium in the gas, and that the outflow of gas through the opening does not alter the equilibrium, then the single-particle distribution function  $f(\mathbf{r}, \mathbf{v})$  will be a Maxwell-Boltzmann distribution:

$$f(\mathbf{r}, \mathbf{v}) = \exp\left(-\frac{U + M\mathbf{v}^2/2}{k_B T}\right), \quad (22)$$

where  $U(\mathbf{r})$  is the potential of the gradient force (2).

If we now assume, as usual, that the rate of outflow of gas is determined by the number of atomic and molecular collisions in the opening, then the relation between the rate of gas outflow with and without a laser near field is

$$\frac{dN}{dt} = \left(\frac{dN}{dt}\right)_0 \frac{\int d^2r \exp(-U(\mathbf{r})/k_B T)}{\pi a^2}, \quad (23)$$

where

$$\left(\frac{dN}{dt}\right)_0 = n_0 \pi a^2 \sqrt{\frac{k_B T}{2\pi M}}$$

is the rate of outflow through the opening in the absence of a field ( $M$  is the mass of the particles, and  $n_0$  is the particle number density far from the opening). From this expression we can find the effective capture cross section introduced in the previous section:

$$S_{\text{eff}} = \int d^2r \exp \left[ - \frac{U(\mathbf{r})}{k_B T} \right]. \quad (24)$$

Here the integral is over the cross section of the opening. From this expression it follows that the rate of outflow is determined by the potential of the gradient force over the opening.

To find the potential of the gradient force over the opening, we can make use of the general expression (4) with  $z=0$ . However, it is simpler to obtain the unknown energy density from the boundary condition on the opening, according to which the normal component of the field vanishes, and the tangential component is given by

$$\mathbf{E}_{\text{tan}}(\mathbf{r}) = 2\pi[\mathbf{n}_z \mathbf{K}], \quad (25)$$

where  $\mathbf{K}$  is the density of the induced surface current and is given by

$$\mathbf{K} = \frac{2ik}{3\pi^2} \left[ 2\mathbf{H}_0 \sqrt{a^2 - r^2} + \frac{\mathbf{H}_0 r^2 - \mathbf{r}(\mathbf{H}_0 \mathbf{r})}{\sqrt{a^2 - r^2}} \right]. \quad (26)$$

Here  $\mathbf{H}_0 = E_{0m} / \sqrt{2}[-i, 1, 0]$  in our case of a circularly polarized wave.

Taking all of the above into account, the mean square of the electric field over the opening is

$$\langle \mathbf{E}^2 \rangle = \left( \frac{2kE_{0m}}{3\pi} \right)^2 \left[ 8(a^2 - r^2) + 4r^2 + \frac{r^4}{2(a^2 - r^2)} \right]. \quad (27)$$

Substituting this expression into the gradient force potential, we can represent the effective capture cross section in the form of the simple integral

$$S_{\text{eff}} = \pi a^2 \int_0^1 dw [1 + \zeta(2 + 5w + 1/w)]^{-\eta_T \Delta/2}, \quad (28)$$

where

$$\zeta = \frac{8G}{1 + \Delta^2} \left( \frac{ka}{3\pi} \right)^2, \quad \eta_T = \frac{\hbar \Gamma}{2k_B T}. \quad (29)$$

This integral cannot be expressed in terms of elementary functions; however, its numerical integration does not present any difficulties. Let us turn our attention now to the fact that for negative frequency offsets (attraction) and low enough temperatures, the integral (28) diverges. This happens because the singularity of the gradient force potential in the vicinity of the boundary of the opening leads to a singularity in the number density and flux of the particles. Here the total number of particles in the vicinity of this singularity becomes infinite at low enough temperatures, which points to the necessity of taking account of additional physical effects. In particular, we cannot take the screen to be infinitesimally thin, and if its thickness is  $d$ , then the singularity vanishes, since the energy density in the vicinity of the boundary of the opening is proportional to  $1/d$ . As a result, we have for the effective cross section

$$S_{\text{eff}} = \pi a^2 \int_{\delta}^1 dw [1 + \zeta(2 + 5w + 1/w)]^{-\eta_T \Delta/2}, \quad (30)$$

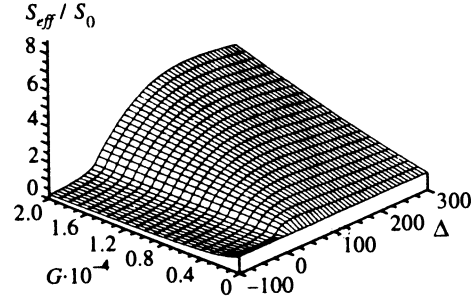


FIG. 7. Relative effective capture cross section of atoms of the equilibrium gas  $\text{Ne}^{20}$  as a function of the relative frequency offset  $\Delta$  of the field in units of  $\Gamma/2$  and the saturation parameter  $G$  for  $\eta_T = \hbar \Gamma / 2k_B T = 0.01$  ( $T = 0.02$  K).

where  $\delta = (d/a)^2$  characterizes the thickness of the screen  $d$ . Here, of course, in order to ensure that our expressions for the laser near field remain valid, the condition  $\delta \ll 1$  must be satisfied.

Figure 7 shows the dependence of the effective cross section of the opening on the intensity of the incident radiation and its relative offset in a gas of  $\text{Ne}^{20}$  atoms at  $T = 0.02$  K ( $\eta_T = 0.01$ ). It is clear from this figure that in the case of a quasi-equilibrium gas illumination of the opening by resonant laser radiation leads to an appreciable change in the rate of outflow.

#### 4. APPLICATION OF THE METHOD. SELECTION OF NOBLE-GAS ISOTOPES

In the foregoing sections we demonstrated that under reasonable and accessible conditions (intensity and frequency of resonant laser light) it is possible to substantially increase the effective capture cross section of particles of the required sort. For this selection method to be usable, it is also necessary that such an increase not taken place for other kinds of particles, in other words, it is necessary that the structure of the transitions of the atoms or molecules that are to be separated differ sufficiently. Thus, the problem reduces to finding spectral lines that differ substantially between the selected and unselected atoms either in frequency or in polarization (enantiomers). Below, in the case of isotopes of noble gases (neon), we demonstrate that selection with the help of a laser near field can be quite effective.

Applying the results of Sec. 2 to a beam consisting of a mixture of  $\text{Ne}^{20}$  and  $\text{Ne}^{22}$ , it is not hard to find a relation between the effective capture cross sections of the two isotopes as a function of the frequency offset ( $G = 1000$ ,  $V_0 = 1$  m/s, for counterpropagating beam and radiation). We consider the transition  $^1S_5^3p_2 \rightarrow ^2P_9^3d_3$  with wavelength 640.2 nm, isotopic shift 1.62 GHz, and total line width  $\Gamma/2\pi = 8 \times 10^6 \text{ s}^{-1}$ . The results of our calculations are shown in Fig. 8 from which it can be seen that effective selection is possible via an appropriate positive offset (relative to  $\text{Ne}^{20}$ ).

We stress again that we are not talking here about a practical implementation of isotope separation, merely about a physical effect. It can also be used for selection of, say, left- and right-handed molecules in a circularly polarized field.

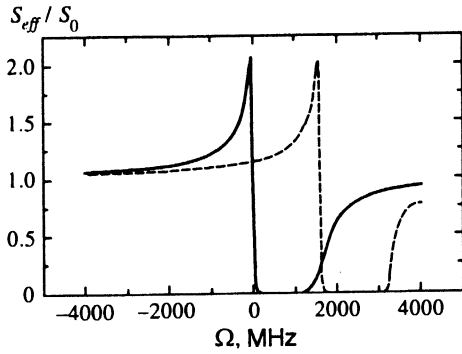


FIG. 8. Effective capture cross section of  $\text{Ne}^{20}$  atoms (solid line) and  $\text{Ne}^{22}$  atoms (dashed line) in a metastable state as functions of the offset of the laser light ( $ka=2$ ,  $\lambda=640.2$  nm,  $G=10^3$ ,  $V_0=1$  m/s).

## 5. CONCLUSION

In the present paper, in the instance of, generally speaking, nonequilibrium systems we have shown that illumination of an opening (or a set of openings), small in comparison with the wavelength, by resonant radiation allows one, in a nondestructive way, to influence a flux of atoms or molecules passing through the opening, and thus to implement selection of neutral atoms and molecules.

An important feature of this effect is its dependence on the direction of travel of the atoms. This is especially pronounced in the passage of an atomic beam through the opening (see Figs. 6a and 6b). The dependence on the direction leads to the idea not only of using this effect to select one type of particle, or another, but also to implement Maxwell's demon, i.e., to separate a mixture of gases with the least possible energy expenditure.

Indeed, consider the scheme shown in Fig. 9. Let an atomic gas be located in two cavities connected by a small opening with radius  $a$ , satisfying the condition

$$r_{\text{at}} \ll a \lesssim \lambda, \quad (31)$$

where  $r_{\text{at}}$  is the characteristic radius of the atom, which for slow atoms is determined not by the radius of the electronic shell, but by the de Broglie wavelength. Under equilibrium

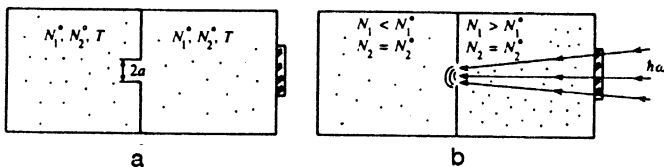


FIG. 9. Scheme for implementing selection of particles in a laser near field.

conditions, i.e., without laser irradiation, the composition, pressure, and temperature for a two-component mixture of atoms are the same in both cavities (Fig. 9a). Now let the small opening be illuminated from one side through an optical window by laser light. It is clear that the total "gas+laser field" system is now far out of equilibrium. If the laser frequency  $\omega$  is in resonance with the quantum transition of atoms of some given kind, then for a negative offset  $\Omega=\omega-\omega_{01}<0$ , the atoms from the field-free region (the region on the left) will have a larger effective capture cross section than the atoms approaching the opening from the right (from the side of the laser light source; see Fig. 9b). As a result, on the left side the number density of the atoms  $N_1$  will be less than its original value  $N_1^0$ ,  $N_1 < N_1^0$ , and conversely, on the right side we will have  $N_1 > N_1^0$ .

This laser version of Maxwell's demon, of course, obeys the second law of thermodynamics. First, energy is transferred from the laser field to the atoms due to recoil when momentum  $\hbar\Delta\mathbf{k}=\hbar(\mathbf{k}_1-\mathbf{k}_2)$  is transferred to an atom. Here  $\mathbf{k}_1$  and  $\mathbf{k}_2$  are the wave vectors of the absorbed and reemitted (stimulated emission) photons, respectively. Second, the entropy of the atomic gas decreases, while the entropy of the light increases. The latter takes place due to fluctuations, not considered here (see Ref. 12), in the number and direction of the reemitted photons. Thus, despite the fact that to a first approximation the dipole (gradient) force is a potential (conservative) force, in the total "gas+unidirectional laser field" system, energy is pumped from the laser field to the atomic gas, and entropy, from the gas to the field.

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