Kinetic Description of Feed-Back Non-Resonant Optical Lattices-Gas Interaction

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Abstract

In this paper the effects of coupling a non-resonant optical lattice to a gas is studied. When the lattice induces a periodic modulation of the gas density, strong Bragg diffraction of light can occur. If a significant fraction of the light used to make the periodic structure is diffracted it can potentially limit the achievable intensities inside the lattice limiting the ability to manipulate the gas with the light. We calculate the evolution of the light fields by finding solutions to the wave equation with a periodic refractive index induced by the lattice. The local gas density perturbation induced by the lattice is determined by solution of the Boltzmann kinetic equation in the collisional regime. This allows us to predict the limits of gas transport within optical lattice. We discuss the maximum energy and momentum transfer to the gas from the lattice.

Introduction

The manipulation of atomic and molecular gases using strong optical fields has applications in the creation of cold molecules by deceleration of cold molecular beams and for measurement of thermodynamic parameters in the gas phase using the techniques of coherent Rayleigh [1,2] and coherent Rayleigh-Brilluoin scattering [3-5]. In all these techniques the dipole force within an optical lattice creates a modulation of the gaseous medium. In optical Stark deceleration, which is used to create slow cold molecules from a molecular beam, the molecules are trapped by the lattice in a periodic structure and transported to a well defined velocity, either by the oscillatory dynamics of the centre-of-mass motion of the trapped particles, or by acceleration or deceleration of the lattice itself. When using this lattice interaction for gas diagnostics, the frequency profile of the light scattered from a periodic modulation of the gas refractive index contains information on the temperature and gas composition. The periodic modulation of the refractive index of the gas leads to the creation of a Bragg structure which efficiently diffracts light when the gas density is large. If a significant fraction of the light used to make the periodic structure is diffracted, it can potentially limit the achievable intensities inside the lattice which could degrade the ability to manipulate of gases the optical lattices. This effect becomes important when a pulsed or continuous optical lattice is produce for acceleration/deceleration, gas separation, local gas heating and microscale gas mixing and other processes, considered in a recent review [6].

In this paper we use a two wave mixing process to produce a self consistent approach to model the interaction between the velocity distribution of the gas and the optical field used to perturb the distribution. The evolution of the gas is modeled as a distribution function, which is perturbed by the dipole force of the optical lattice. The local density and thus the refractive index variation of the gas in the lattice can be determined which controls the diffraction of the light. The evolution of the diffracted light field and the lattice beams is determined by solution of the wave equation.

The evolution of electric field, E, of the light within the lattice in space, x, and time, t, is determined by solution of the wave equation [7],

$$\frac{\partial^2 E}{\partial x^2} - \frac{n^2}{c^2} \frac{\partial^2 E}{\partial t^2} = \mu_0 \frac{\partial^2 P_{nl}}{\partial t^2} \tag{1}$$

where *n* is the refractive index, *c* is the speed of light, μ_0 is the permeability of free space and P_{nl} is non-linear polarizability of the medium.

When operated far from resonance, the refractive index can be related to the polarizability of the gas particles by

$$n = \sqrt{1 + \frac{N\alpha}{\varepsilon_0}} \approx n_0 + \Delta n(x, t)$$
⁽²⁾

The refractive index of the unperturbed gas is $n_0 = 1 + \frac{N_0 \alpha}{2\varepsilon_0}$ where N₀ is the unperturbed gas density and

 α is the static polarisability of each particle. The perturbation of the refractive index induced by the field is related to the change in density and is given by

$$\Delta n(x,t) = \frac{\Delta N(x,t)\alpha}{2\varepsilon_0}; \ \left|\Delta n\right| << n_0 \tag{3}$$

If we assume that the scattering process is only due to spatial organization of the gas only the linear polarizability is important and thus we can neglect the nonlinear polarizability term in equation (1) such that

$$\frac{\partial^2 E}{\partial x^2} - \frac{n_0^2}{c^2} \frac{\partial^2 E}{\partial t^2} = \frac{2n_0 \Delta n}{c^2} \frac{\partial^2 E}{\partial t^2}$$
(4)

The gas density perturbation, $\Delta N(x,t)$, can be found from the velocity distribution function as

$$\Delta N(x,t) = \int_{-\infty}^{\infty} [f(x,v,t) - f_0] dv, \ N_0 = \int_{-\infty}^{\infty} f_0 dv$$
(5)

where $f_0(v,T)$ is the local Maxwellian distribution function and f(x,v,T) is derived by solution of the 1-D Boltzmann equation along the lattice direction, *x*, given below.

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{F(x,t)}{m} \frac{\partial f}{\partial v} = -\frac{f - f_0}{\tau_c}.$$
(6)

We need only consider the fields and gas motion in 1-D along the x direction as the axial force which induces the refractive index change is much stronger than the radial force. As we use pulsed light fields no radial motion is induced and therefore does not affect the diffracted radial field components. We consider the collisional term of the Boltzmann equation to be, $-(f - f_0)/\tau_c$, in the Bhatnagar-Gross-Krook (BGK) approximation [8] as we assume our perturbations are small.



Fig. 1. Schematic of 1D laser beams interference pattern.

Figure 1 shows the input and output fields that interact with the gas to produce a periodic refractive index structure Bragg structure. The optical lattice is created by the interference of two plane waves of intensities I_1 and I_2 (Fig. 1) with electric fields

$$E_1 = A_1 \exp[i(k_1 x - \omega_1 t)] + \text{c.c.} \quad ; \quad E_2 = A_2 \exp[i(k_2 x + \omega_2 t)] + \text{c.c}$$
(7)

The phase velocity of the interference pattern and the slowly varying field amplitude in the interference region are

$$\xi = (\omega_1 - \omega_2)/(k_1 + k_2) = \Omega/q,$$
(8)

where ω_1, ω_2 and k_1, k_2 are the frequencies and wavevectors of each field. The intensity is proportional the square of the field given by

$$E^{2}(x,t) = E_{01}(x,t)E_{02}(x,t)\cos(qx - \Omega t)$$
(9)

where $E_{01,2}(x,t) = 2[A_{1,2}(x,t)A_{1,2}^*(x,t)]^{1/2}$.

Note, that a standing or moving optical lattice can conceptually be created by a single laser and a standing or moving mirror [6].

For molecules that are far detuned from resonance, the optical lattice/electrostrictive potential is given in the quasi- electrostatic approximation described by [7]

$$U(x,t) = -\frac{1}{2}\alpha E^{2}(x,t)$$
(10)

The gradient (or ponderomotive) force along the lattice is given by:

$$F(x,t) = -\frac{\partial U(x,t)}{\partial x}$$

$$= \frac{\alpha}{2} \left(\frac{\partial E_{01}}{\partial x} E_{02} + \frac{\partial E_{02}}{\partial x} E_1 \right) \cos(qx - \Omega t) - \frac{\alpha}{2} E_{01} E_{02} q \sin(qx - \Omega t)$$
(11)

The perturbation of the index of refraction, which leads to Bragg diffraction for the case where $\Delta n \propto \Delta N$ is given by

$$\Delta n = 0.5 \Delta n_a \{ \exp[i(k_1 + k_2)x - (\omega_1 - \omega_2)t] + c.c. \}.$$
(12)

The evolution of the fields is simplified using the slowly varying envelope approximation, which is valid when the field envelope varies slowly compared to the optical frequency. These approximations are given as

$$\frac{\partial^2 A_{1,2}}{\partial x^2} << k_{1,2} \frac{\partial A_{1,2}}{\partial x} << k_{1,2}^2 A_{1,2}; \frac{\partial^2 A_{1,2}}{\partial t^2} << \omega_{1,2} \frac{\partial A_{1,2}}{\partial t} << \omega_{1,2}^2 A_{1,2}.$$
(13)

From the optical wave equation (4), the equation for E^2 (9) and for refractive index variation induced by the fields (12), we derive the equations for the complex electric field in each interacting laser beam:

$$\frac{\partial A_1}{\partial t} + \frac{c}{n_0} \frac{\partial A_1}{\partial x} = -\frac{\Delta n_a \omega_2}{\omega_1 n_0} \frac{\partial A_2^*}{\partial t} + i \frac{\Delta n_a \omega_2^2 A_2^*}{2\omega_1 n_0}$$
(14a)

$$\frac{\partial A_2}{\partial t} - \frac{c}{n_0} \frac{\partial A_2}{\partial x} = -\frac{\Delta n_a \omega_1}{\omega_2 n_0} \frac{\partial A_1^*}{\partial t} - i \frac{\Delta n_a \omega_1^2 A_1^*}{2\omega_2 n_0}$$
(14b)

These equations describe the conversion of one field on the right hand side of equations 14 into the other field on the left hand side of these equations. That is one field is diffracted by the refractive index grating and becomes part of the other counter-propagating field that forms the grating. We can simplify these equations even further by realizing that the gas parameters are changing on a much slower time scale than the field amplitudes and then equations 14 are transformed to

$$\frac{dA_1}{dx} = i \frac{\Delta n_a \omega_2^2 A_2^*}{2\omega_1 c}$$
(15a)

$$\frac{dA_2}{dx} = i \frac{\Delta n_a \omega_1^2 A_1^*}{2\omega_2 c}$$
(15b)

at each time step. For a gas interaction length L, the boundary conditions for field amplitudes are given by $A_1(0,t) = A_1^*(0,t) = \sqrt{I_1(0,t)/2\varepsilon_0 c}$; $A_2(L,t) = A_2^*(L,t) = \sqrt{I_2(0,t)/2\varepsilon_0 c}$ (16)

Analytical solution

We can now obtain an analytical solution for the field amplitudes as a function of position along the induced Bragg grating. At $\Delta n_a(x) = \text{const}$, we can find the analytical solution of equations (15a) and (15b) satisfying the boundary conditions (16) given by

$$A_{1}(x) = \frac{A_{1}(0)\cosh[s(x-L)]}{\cosh(sL)} + i\frac{A_{2}(L)\sqrt{\omega_{2}^{3}/\omega_{1}^{3}}\sinh(sx)}{\sinh(sL)},$$
(17a)

$$A_{2}(x) = \frac{A_{2}(L)\cosh(sx)}{\cosh(sL)} - i \frac{A_{1}(0)\sqrt{\omega_{1}^{3}/\omega_{2}^{3}}\sinh[s(x-L)]}{\cosh(sL)},$$
(17b)

where parameter $s = \Delta n_a (\omega_1 \omega_2)^{1/2} / 2c$.

Numerical solution

In general case when the index refraction perturbation is position and time dependent ($\Delta n = \Delta n(x,t)$), we can find a numerical time-dependent solution. For a known index of refraction perturbation with an amplitude $\Delta n_a(x,t)$, determined at each "gasdynamic" time step, we solve equations (15a), (15b) with

boundary conditions (16), using the second-order Euler scheme. Because the boundary conditions for complex field amplitudes (16) correspond to the opposite sides of the interaction region, the iteration procedure is applied up to complete convergence of all unknown parameters with given high accuracy. Afterwards, a corresponding distribution for the ponderomotive force (11) was computed and a new value of the distribution function $f(x,t+\Delta t)$ was then calculated from the Boltzmann equation (6) with the ponderomotive force (11). The Boltzmann equation (6) was solved using a 2nd order McCormack predictor-corrector method [9]. The density perturbation (5) and corresponding index refraction perturbations (3) were defined.

Traveling Bragg lattice

The interaction of laser beams with the OL-induced gas periodic density perturbation results in Bragg scattering (Fig. 2). When the phase velocity (8) $\xi \ll c$ in the reference frame of the traveling Bragg lattice the incident and reflected waves are Doppler shifted by $\omega_{1,f} = \omega_1(1-\xi/c)$ and $\omega_{1,R} = \omega_1(1-2\xi/c) \approx \omega_2$.

The same happens for the other incident wave, $\omega_{2,R} \approx \omega_1$.



Fig. 2. Schematic of interaction with self-consistent traveling Bragg lattice

Optical field-gas energy conservation

The density of energy dissipation power is given by:

$$\frac{\partial W_g(x,t)}{\partial t} = \int_{-\infty}^{\infty} F(x,t) f(x,v,t) v dv , [W/m^3]$$
(18)

The total dissipation rate in a gas for a cylindrical interaction region of length L and cross-section S is given by

$$P_g = \frac{d}{dt} \int_V W_g dV = S \int_0^L \left[\int_{-\infty}^{\infty} F(x,t) f(x,v,t) v dv \right] dx , [Watt]$$
(19)

In agreement with the conservation of energy, described by the general conservation of energy equation [10]. The change of energy stored in a gas is related to the dissipation of the laser radiation energy given by

$$\frac{\partial W_E}{\partial t} + \vec{\nabla} \cdot \vec{\Pi} = -\frac{\partial W_g}{\partial t} \,. \tag{20}$$

Here $W_E(x,t)$ is the density of the electromagnetic energy averaged over the period of optical field

$$W_{E}(x,t) = \left\langle \frac{\varepsilon_{0}\varepsilon(\vec{E}_{1}+\vec{E}_{2})^{2}+\mu_{0}\mu(\vec{H}_{1}+\vec{H}_{2})^{2}}{2} \right\rangle_{2\pi/\omega_{1,2}}$$

$$\approx \varepsilon_{0}\varepsilon \left(\frac{E_{01}^{2}}{2}+\frac{E_{02}^{2}}{2}+E_{01}E_{02}\cos(qx-\Omega t)\right) = ; \quad (21)$$

$$= \frac{I_{1}}{c}+\frac{I_{2}}{c}+\frac{2(I_{1}I_{2})^{1/2}}{c}\cos(qx-\Omega t)$$
and $\vec{\Pi} = \vec{E} \times \vec{H}$, (22)

is the Poynting vector [10, 11]. The averaged Poynting vector is $\langle \vec{\Pi}_{1,2} \rangle_{2\pi/\omega_{1,2}} = I_{1,2}\vec{i}_{1,2}$, where $\vec{i}_{1,2}$ is the unit vectors in the direction of wave propagation. Integrating of eq. (20) over the whole interaction volume gives

$$P_{EM} + \oint_{S} \vec{\Pi} d\vec{S} = -P_{g}, \qquad (23)$$

where $P_{EM} \equiv \frac{d}{dt} \int W_E dV = \frac{d}{cdt} \int (I_1 + I_2) dV$ is the rate of dissipation of electromagnetic energy. From (23) it follows the balance of Poynting vector fluxes is

 $\Delta \Pi = I_1(0,t) - I_1(L,t) + I_2(L,t) - I_2(0,t) = -(P_{EM} + P_g)/S.$ (24)

Momentum transferred from the OL to the gas

In general case, the rate of changing of the x-projection of momentum (force in x-direction) [11] is

$$\frac{d}{dt}(\vec{\Xi}_{gas} + \frac{1}{c^2} \int_{V} \vec{\Pi} dV)_x = \oint_{S} T_{xn} dS_n, \qquad (25)$$

where $\Xi_{gas} = mS \int_{0-\infty}^{L} \int_{0-\infty}^{\infty} f(x,v,t) v dv dx$ is the instantaneous momentum of the gas and $\frac{1}{c^2} \int_{V} \vec{\Pi} dV$ is the total

momentum of the electromagnetic field in the OL volume, correspondingly; T_{ij} is the Maxwell stress tensor:

$$T_{ij} = E_i D_j + H_i B_j - \frac{1}{2} \delta_{ij} E_k D_k - \frac{1}{2} \delta_{ij} H_k B_k \,.$$

If the OL is created by the interference of two opposite plane waves with $\vec{E}_{1,2}(0, E_{1,2y}, 0)$ and $\vec{H}_{1,2}(0, 0, H_{1,2z})$, the tensor along the lattice is $T_{xx} = -\frac{1}{2} \varepsilon_0 \varepsilon E_y^2 - \frac{1}{2} \mu_0 \mu H_z^2$. The averaged value over laser field period is

(26)

$$< T_{xx} >_{2\pi/\omega} = -\frac{1}{2} \varepsilon_0 \varepsilon E_{0y}^2 = -\frac{I}{c}$$
. The momentum transferred to gas by the pulsed OL of duration $\tau >> 2\pi/\omega_{1,2}$ is

$$\Xi_{gas,x} = \int_{0}^{\infty} \oint_{S} \langle T_{xx} \rangle_{2\pi/\omega} \, dSdt = \frac{S}{c} \int_{0}^{\infty} \left[I_1(0,t) - I_1(L,t) - I_2(L,t) + I_2(0,t) \right] dt.$$
(27)
For the rectangular pulse of τ duration the momentum of the gas is

$$\Xi_{gas,x} = (S/c)[I_1(0) - I_1(L) - I_2(L) + I_2(0)]\tau.$$
⁽²⁸⁾

Example Results

I. An amplifier

In the case of two equal opposite laser beams, the result of optical lattice-gas interaction is symmetric. The Bragg lattice induced in result of optical lattice - gas interaction is self-consistent and the beam reflected back comes to the beam of opposite direction. Therefore, it is possible to amplify a weak laser beam interfering with intensive beam, because of reflection back of a high intensity beam results in a relatively strong amplification of the weak intensity beam.



Fig. 3. Longitudinal distribution of the weak beam intensity along the optical lattice: amplifying of the weak intensity beam (right). Red - results for self-consistent calculations by complete set of equtions; dashed – analytical solution for numerically obtained amplitude for the perturbation of index of refraction, Δn_a determined by equations (17a) and (17b). The interaction region length is taken as $L = 200\lambda$.

An example of interaction of two interfering laser beams is considered for methane gas at p=1 Atm and T=293 K with equal laser beam intensities $I_1(0) = 10^{16}$ and $I_2(L) = 10^{12}$ W/m². Let, for example, the laser wavelength to be $\lambda = 532$ nm and the frequencies of each beam are equal giving a lattice phase velocity, $\xi = 0$. The results for amplifier are shown in Fig. 4 and 5. Fig. 4 shows the longitudinal distribution of the weak beam intensity along the optical lattice illustrating the amplification of the weak beam as it propagates from right to the left.

It is clear that the effect of amplification is stronger the larger the difference between the beam intensities and the longer the interaction length. For optical lattice of $L = 10^4 \lambda = 0.532$ and $2 \cdot 10^4 \lambda = 1.064$ cm a simple parabolic extrapolation gives an amplification of $I_2(0)/I_2(L) = 2.33$ and 6.36 correspondingly.

A similar analysis for energy transfer from one laser beam to another made for co-propagating timedependent laser beams that are intersecting in liquids is given in reference [12].

II. Gas - OL self-consistent interaction

The results for CH₄ gas for the case of $I_1(0) = I_2(L) = 5 \times 10^{15}$ W/m²; p=10 Torr; T₀=293 K; $\lambda = 532$ nm and L=100 λ are shown in Figures 5-8. At relatively low gas density ($\lambda_{OL}/l_c \sim 1$) modulation of the laser beam intensity results because of the gas bouncing between the walls of the optical lattice.

Presented results clearly show that all parameters are modulated with the period determined by the sobounce The called frequency. bounce frequency for trapped particles is $\Omega_{\rm B} \approx q \sqrt{U/2m}$ where $U = 2\alpha I/\varepsilon_0 c$. The estimated frequency is $\Omega_B \approx 3.37 \times 10^9$ rad/s and $T_{B} = 2\pi / \Omega_{B} \approx 1.86$ ns are in very good agreement with the computed data. The amplitude of oscillation is decaying due to collisions at the given conditions (10 Torr, 293 K) equal to $\tau_c = 8$ ns. Results of optical lattice – gas interaction depend on OL phase velocity. At $\xi \neq 0$, the plateau forms a distribution with the half-width $\Delta v = (2U/m)^{1/2}$ shown in Fig. 7.



Fig.5. Powers per unit optical lattice cross-section, P_{EM} , P_g and Poynting vector balance, $\Delta \Pi$. Left: at phase velocity $\xi = (2kT/m)^{1/2}$; Right: $\xi = -(2kT/m)^{1/2}$



Fig.6. Gas velocity averaged over the lattice wave length. Left: at phase velocity $\xi = (2kT/m)^{1/2}$; Right: $\xi = -(2kT/m)^{1/2}$



Fig.7. Distribution functions at OL phase velocities $\xi = \pm (2kT/m)^{1/2}$.

Because of presence of collisions there is dissipation, even at $\xi = 0$ (Fig.8)



Fig.8. Powers per unit optical lattice cross-section (top, left), changing of relative intensities for left and right beams (top, right) and distribution function (bottom) at t=10 ns. The phase velocity is $\xi = 0$.

Dissipation of laser power in a gas

It is interesting to compare results for laser power absorption in a gas, computed with eq. 18, with a simplified analytical solution that was derived in [13,14]. The power absorbed in the gas is

$$\mathbf{W}_{g} \approx \frac{2m^{2}\xi^{2}}{\lambda kT} f_{0}(\xi,T) \Delta^{4} = \frac{8\xi^{2}}{\lambda kT} f_{0}(\xi,T) U^{2}; \ \Delta = (2U/m)^{1/2}; \ U = 2\alpha I/\varepsilon_{0}c$$
(26)

We make a comparison at the following conditions where the gas is CH₄, the pressure is p=760 Torr and the laser intensities are $I_1(0) = I_2(L) = 10^{16}$ W/m² and the wavelength is $\lambda = 532$ nm. Both the analytical theory and the results of numerical calculations (Fig. 9) give the same dependence with intensity $\dot{W}_g \propto I^2$. The maximal absorption rate at phase velocity $\xi = (2kT/m)^{1/2}$ is in good quantitative agreement.



Fig.9. Comparison of simplest analytical [14] and detailed computations with the present model. Both predict the same phase velocity for maximum absorption. In both the power absorbed scales as l^2 .

Conclusions

In this paper we studied the non-linear interaction of an optical lattice with a gas on the basis of the Maxwell equations for the laser fields and the Boltzmann kinetic equation for gas motion in low and high density cases. As a result of induced gas density (and therefore the index of refraction) perturbation, the Bragg lattice forms resulting in feed back of the laser radiation. The strength of interaction depends on optical lattice phase velocity. It is shown that if the relative intensities of opposite laser beams are very different then amplification of weaker beams is possible. At relatively low gas densities, when the free mean path is comparable with the optical lattice wavelength, we predict the modulation of the generated laser beam intensities, which occurs due to energy and momentum exchange with the trapped bouncing gas and the field. Generalized equations for the optical field-gas energy and momentum conservation were also presented.

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