Three-dimensional analysis of the magneto-optical trap for (1+3)-level atoms

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We describe a three-dimensional model of the magneto-optical trap (MOT) for the simplest case of (1+3)-level atoms. The atomic density matrix equations are solved up to eighth order in the Rabi frequency and compared with experimental observations. We propose that coherences between the excited state sublevels can largely explain the dependence of the atomic temperature on detuning and light intensity.

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I. INTRODUCTION

The cooling and trapping of atoms in a magneto-optical trap (MOT) has been studied extensively in past years [1]. Different kinds of MOTs have found applications in optical and microwave spectroscopy, atomic and optical physics, and atomic clocks. More recently, MOTs for even isotopes of alkaline-earth atoms such as ^{24}Mg, ^{40}Ca, ^{88}Sr, and ^{174}Yb have been proposed as a promising way to develop optical lattice clocks with an accuracy of 10^{-17} [2–5].

The dipole interaction of the above atoms with the MOT light field can be described by a (1+3)-level atomic model with Zeeman-shifted upper-state sublevels. The first example of this model was a one-dimensional (1D) interaction scheme which obtained expressions for the potential depth, the friction coefficient, and momentum diffusion coefficients [6]. It was found that at low laser intensity the damping coefficient in the 1D (1+3)-level interaction scheme is close to that derived from the 1D theory of Doppler cooling for two-level atoms [7]. Hence experimental results for laser cooling of (1+3)-level atoms in this regime are usually compared with predictions based on the 1D theory for two-level atoms.

For an MOT operating at high laser intensity, the measured temperature of (1+3)-level atoms has been found to be significantly higher than expected from the 1D two-level Doppler cooling model [8–12]. Various mechanisms have been proposed to explain the additional heating. Inelastic collisions can induce heating, but this mechanism becomes significant only at atomic densities higher than typical for MOTs [13]. Another mechanism is driven by transverse spatial intensity fluctuations. An investigation of a 1D configuration for cooling ^{88}Sr has shown that molasses intensity imbalances can be the dominant cause for extra heating [14].

However, ^{88}Sr atoms trapped in an MOT have been measured to be at temperatures above the Doppler limit even when intensity imbalances are largely absent [8,9]. This indicates the presence of yet another mechanism for additional heating of (1+3)-level atoms. One possible explanation considers the role of coherences between the sublevels of the excited state [15]. The quantitative contribution of these coherences to the atomic temperature has remained an open question for realistic experimental schemes. The difficulty lies in the three-dimensional (3D) complexity of the optical processes responsible for atomic excitation in an MOT. To our knowledge, only one *ab initio* 3D MOT theory for (1+3)-level atoms has been published in the literature [16]. The theoretical treatment in Ref. [16] is however restricted to the case of low light intensity and does not consider coherences between the upper-state sublevels. The result is an atomic temperature that agrees with the expectation from the 1D Doppler theory for two-level atoms.

In this paper, we present a 3D model of the MOT for the simplest nontrivial case of (1+3)-level atoms. Our theory is a 3D extension of previous *ab initio* calculations for 1D laser cooling of atoms in an MOT [17,18]. In particular, it includes contributions from upper-state coherences to the atomic temperature which become significant as the light intensity increases. Section II describes our 3D MOT model for (1+3)-level atoms. Steady-state solutions for the friction force, diffusion coefficients, and the atomic temperature are given in Sec. III. In Sec. IV, the results from our 3D theory for the atomic temperature are compared with the 1D case and experimental observations. Section V concludes with a summary and discussion.

II. 3D ATOMIC MODEL

We choose a standard geometry for the magnetic field near the center of the MOT [1]:

$$\mathbf{B} = -\frac{a}{2}(x\mathbf{e}_x + y\mathbf{e}_y - 2z\mathbf{e}_z), \tag{1}$$

where a is the magnetic field gradient at the trap center $\mathbf{r}=0$. The 3D light field consists of three pairs of counter-

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propagating circularly polarized waves. In the laboratory frame, the total field can be written as

$$\mathbf{E} = \sum_{j=x,y,z} \mathbf{E}^{(j)} + \mathbf{E}^{(-j)}, \tag{2}$$

where the electric fields of the circularly polarized waves written in standard notation [19] are

$$\mathbf{E}^{(j)} = \frac{1}{2} E_0 (\mathbf{e}_-^j e^{i(kj-\omega t)} - \mathbf{e}_+^j e^{-i(kj-\omega t)}),$$

$$\mathbf{E}^{(-j)} = \frac{1}{2} E_0 (\mathbf{e}_+^j e^{-i(kj+\omega t)} - \mathbf{e}_-^j e^{i(kj+\omega t)}). \tag{3}$$

Each pair of the laser fields $\mathbf{E}^{(j)}+\mathbf{E}^{(-j)}$ represents a $\sigma^+-\sigma^-$ field configuration, and their polarizations are defined by spherical unit vectors.

The atomic Hamiltonian can be written as [18]

$$H = H_0 - (\hbar^2/2M)\boldsymbol{\nabla}^2 - \boldsymbol{\mu}\cdot\mathbf{B} - \mathbf{d}\cdot\mathbf{E}, \tag{4}$$

where H_0 describes the internal atomic states, the second term is the kinetic energy operator, and the last two terms describe the dipole interaction of the atom with the magnetic field and the light field, respectively. The atom is assumed to have total angular momentum quantum number $F_g=0$ in the ground state and $F_e=1$ in the excited state. The Rabi frequency Ω is defined as

$$\Omega = \frac{\|d\|E_0}{2\sqrt{3}\hbar}, \tag{5}$$

where $\|d\|$ is the reduced dipole matrix element for the transition between the states $F_g=0$ and $F_e=1$. The spontaneous decay rate W_{sp} of the upper-state magnetic sublevels and the detuning δ of the light field are defined as

$$W_{\mathrm{sp}} = 2\gamma = \frac{4\|d\|^2\omega_0^3}{9\hbar c^3} \quad \delta = \omega - \omega_0, \tag{6}$$

where ω_0 is the atomic transition frequency in the absence of the magnetic field.

Equations (1)–(6) and a standard set of atomic density matrix equations [19] lead to explicit equations for the density matrix elements ρ_{kl} that describe the dipole interaction of a (1+3)-level atom with a 3D light field. The kinetic equation for the Wigner function $w(\mathbf{r},\mathbf{p},t)=\rho_{gg}+\rho_{-1-1}+\rho_{00}+\rho_{11}$ is derived by a standard procedure [19].

Let us consider the atomic motion in the MOT on a spatial scale that exceeds the optical wavelength. In this case the kinetic equation for $w=w(\mathbf{r},\mathbf{p},t)$ considered to second order in the photon momentum $\hbar k$ assumes the form of a Fokker-Planck equation [19],

$$\frac{\partial w}{\partial t} + \mathbf{v}\frac{\partial w}{\partial \mathbf{r}} = -\frac{\partial}{\partial \mathbf{p}}(\mathbf{F}^0 w) + \sum_{j=x,y,z} \frac{\partial^2}{\partial p_i \partial p_j}(D_{ij}^0 w), \tag{7}$$

where $\mathbf{F}^0$ is the spatially averaged radiation force and the spatially homogeneous momentum diffusion tensor is defined by D_{ij}^0.

III. FRICTION, DIFFUSION, AND TEMPERATURE

For negative detuning near the trap center, the velocity-dependent force $\mathbf{F}^0=\mathbf{F}(\mathbf{v})$ reduces to the friction force

$$\mathbf{F}(\mathbf{v}) = -M\beta\mathbf{v}, \tag{8}$$

where M and β are the atomic mass and the friction coefficient, respectively. The friction force is calculated to eighth order in the Rabi frequency (fourth order in the saturation parameter G) to account for the multiphoton processes that contribute to the force near zero velocity [17]. Then the friction coefficient is found to be

$$\beta = \frac{\hbar k^2}{M}\frac{4G(|\delta|/\gamma)}{(1+\delta^2/\gamma^2)^2}\left(1 - \frac{14G}{1+\delta^2/\gamma^2} + \frac{15}{8}\frac{(65-3\delta^2/\gamma^2)G^2}{(1+\delta^2/\gamma^2)^2} - \frac{1}{8}\frac{(10434-905\delta^2/\gamma^2)G^3}{(1+\delta^2/\gamma^2)^3}\right), \tag{9}$$

where

$$G = \frac{2\Omega^2}{\gamma^2} = \frac{\|d\|^2 E_0^2}{6\hbar^2\gamma^2}. \tag{10}$$

Next, the diagonal components of the diffusion tensor are evaluated at the center of the trap and at zero velocity. To the eighth order in the Rabi frequency $D_{ii}^0=D$ becomes

$$D = 2\hbar^2 k^2 \gamma \frac{G}{1+\delta^2/\gamma^2}\left(1 - \frac{21}{4}\frac{G}{1+\delta^2/\gamma^2} + \frac{93}{2}\frac{G^2}{(1+\delta^2/\gamma^2)^2} - \frac{1769}{4}\frac{G^3}{(1+\delta^2/\gamma^2)^3}\right). \tag{11}$$

The atomic temperature can be estimated by applying Eqs. (9) and (11) to the standard relation

$$T = \frac{D}{Mk_B\beta}, \tag{12}$$

which gives an estimate for the temperature valid up to sixth order in the Rabi frequency,

$$T = \frac{\hbar\gamma}{2k_B}\left(\frac{\gamma}{|\delta|} + \frac{|\delta|}{\gamma}\right)\left(1 + \frac{35G}{4(1+\delta^2/\gamma^2)} + \frac{(377+45\delta^2/\gamma^2)G^2}{8(1+\delta^2/\gamma^2)^2} + \frac{(14571+475\delta^2/\gamma^2)G^3}{32(1+\delta^2/\gamma^2)^3}\right). \tag{13}$$

At low saturation, the temperature is reduced to a well-known formula initially derived for two-level atoms [19],

$$T = \frac{\hbar\gamma}{2k_B}\left(\frac{\gamma}{|\delta|} + \frac{|\delta|}{\gamma}\right). \tag{14}$$

According to Eqs. (9)–(13), our perturbation approach converges for any detuning if the saturation parameter $G<1$, i.e., when the light field intensity is less than the saturation intensity.

IV. COMPARISON WITH 1D AND EXPERIMENT

An analytical evaluation of the temperature at high intensities meets considerable difficulties due to the large number

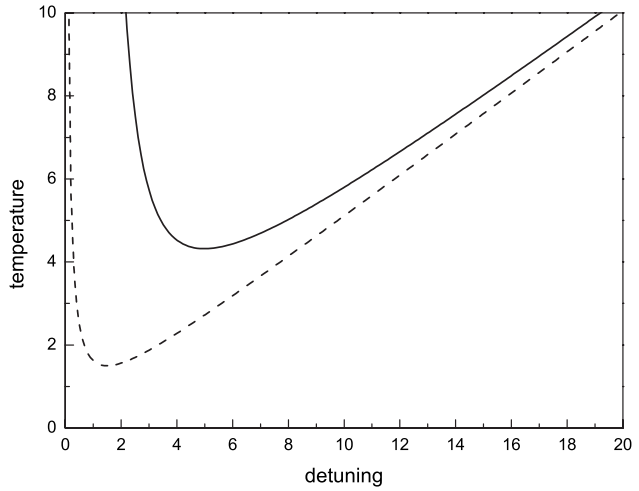

FIG. 1. Atomic temperature $k_B T/\hbar\gamma$ as a function of detuning $|\delta|/\gamma$ at saturation parameter $G=1$. The 3D case (solid line) is calculated to third order in G; the 1D case is exact (dashed line).

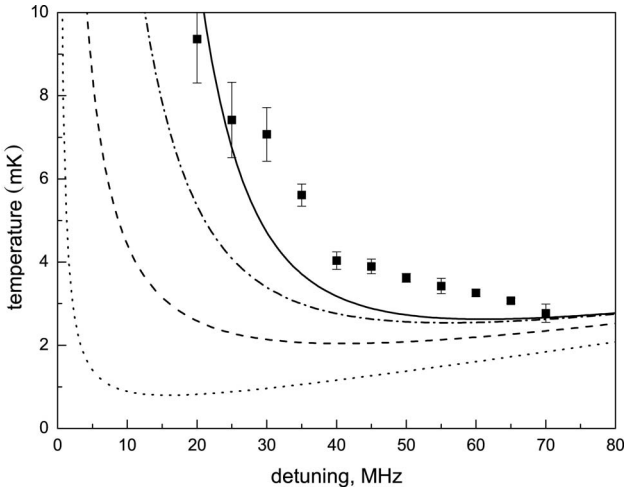

FIG. 2. Experimental dependence of atomic temperature on detuning (Ref. [9]) at $G=0.64$ compared with 3D theoretical curves in zero order (dotted line), to first order (dashed line), to second order (dotted-dashed line), and to third order (solid line) in G.

of spatial harmonics generated by multiphoton processes. This difficulty does not exist in the 1D model, for which the temperature can be calculated exactly at an arbitrary intensity of the light field. It is instructive to compare our 3D results with those from the 1D model.

The 1D case follows directly from the density matrix equations if one assumes that the light field consists of a single $\sigma^+ - \sigma^-$ field configuration. The exact solution of the density matrix equations at the trap center in a one-dimensional field gives the friction coefficient as

$$\beta = \frac{\hbar k^2}{M} \frac{4G(|\delta|/\gamma)}{(1+\delta^2/\gamma^2+2G)(1+\delta^2/\gamma^2+G+G^2/4)}, \quad (15)$$

and the diffusion coefficient at zero velocity as

$$D = \hbar^2 k^2 \gamma \frac{2G}{1+\delta^2/\gamma^2+2G}. \quad (16)$$

Therefore, the atomic temperature is

$$T = \frac{\hbar\gamma}{2k_B} \frac{1+\delta^2/\gamma^2+G+G^2/4}{|\delta|/\gamma}. \quad (17)$$

For sufficiently low light intensity, the temperature shown in Eq. (17) converges to the value found in the 3D model. When G becomes larger, the two models exhibit a difference in temperature behavior as a function of detuning, as shown in Fig. 1. The temperature in the 3D case grows faster as detuning is decreased mainly because its diffusion coefficient increases at a higher rate.

The validity of our 3D MOT theory for (1+3)-level atoms is tested by comparing with experimental data in the published literature that indicate an additional, previously unconsidered heating mechanism [8,9]. In these experiments, ^{88}Sr atoms are excited in an MOT by a laser field with wavelength $\lambda=461$ nm resonant to the dipole transition $^1S_0 - {}^1P_1$. The radiative lifetime $\tau=5$ ns for the excited state corresponds to the natural linewidth $2\gamma/2\pi=32$ MHz. Figures 2 and 3 compare the atomic temperature data of Refs. [8,9] with the temperature calculated from Eq. (13).

Figure 2 shows that the theoretical dependence of the temperature on detuning approaches the experimental data as the perturbation series is successively expanded to higher orders. The convergence rate of the successive theoretical curves to the experimental data is relatively slow since the value of $G=0.64$ in Fig. 2 is fairly large. The dependence of the temperature on the saturation parameter G is shown in Fig. 3. For $G<1$, successive increases in the order of the perturbation series expansion indicate convergence of theory to experimental data. However, our 3D MOT model breaks down for $G \geq 1$ and the convergence disappears.

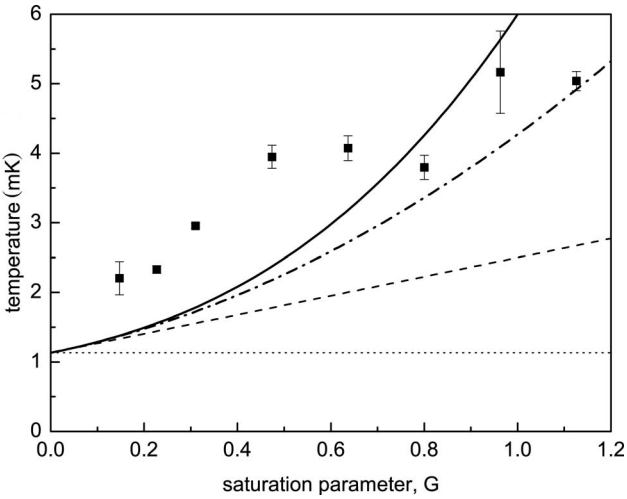

FIG. 3. Experimental dependence of atomic temperature on saturation parameter G (Ref. [8]) at detuning $\delta=-2.5\gamma$ compared with 3D theoretical curves in zero order (dotted line), to first order (dashed line), to second order (dotted-dashed line), and to third order (solid line) in G.

V. CONCLUSION

We have developed a 3D model of the MOT for the simplest case of $(1+3)$-level atoms and compared its predictions with experimental observations. The model applies a perturbation series expansion with respect to the saturation parameter G to solve a Fokker-Planck equation. The analytical treatment takes into account the dipole interaction of the atoms with a 3D field, hence includes multiphoton processes responsible for coherences between the upper-state sublevels. In the limit of small G, the friction force and the diffusion tensor are essentially the same as those obtained from the 1D Doppler theory for two-level atoms. But as G increases, new terms due to numerous multiphoton processes contribute to the upper-state coherences which affect the friction force, the diffusion coefficients, and thus increase the atomic temperature.

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