Monte Carlo Wave-Function Analysis of 3D Optical Molasses

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A full quantum treatment of laser cooling in three dimensions is performed. It is based on a recently developed Monte Carlo wave-function technique, which reduces an otherwise unmanageable density matrix problem by at least a factor of 10^4 in computing requirements. For different atomic transitions and temporal phases of the laser beams, our calculated mean kinetic energies are in good agreement with experimental results. Momentum distributions are shown to develop escape lines when the optical molasses is close to disintegration. Spatial distributions are also calculated and discussed.

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By laser cooling it is possible to obtain samples of atoms with kinetic energies in the microkelvin range [1,2]. The underlying mechanisms have been identified in one-dimensional (1D) models [3,4] in which the atomic center-of-mass motion, subject to fluctuating radiative forces, is treated classically. This led to the scaling law for the atomic mean kinetic energy $E_K \propto \hbar|\delta|s$, where δ denotes the (negative) detuning of the laser frequency with respect to the atomic transition frequency $\delta = \omega_L - \omega_A$. We have introduced the saturation parameter $s = 2|\Omega|^2/(4\delta^2 + \Gamma^2)$, where Γ is the decay rate of the excited state and Ω is the Rabi frequency (atom-laser coupling amplitude). The same scaling laws are found when this semiclassical analysis is applied to cooling in three dimensions [5–8], and in treatments taking proper account of spatial localization, even quantitative agreement with experiments is observed [7].

This treatment does not apply in too weak laser fields, where the measured temperatures increase abruptly after going through a minimum. A quantum formulation of the problem leads [9], in the limit of large detunings, to a universal law for the mean kinetic energy,

$$E_K/E_{\mathrm{Rec}} = f(\hbar|\delta|s/2E_{\mathrm{Rec}}), \tag{1}$$

where the recoil energy, $E_{\mathrm{Rec}} = (\hbar k)^2/2M$, has been introduced, with k being the laser wave number and M the atomic mass. The function f depends only on the angular momentum quantum numbers of the atomic transition and on the laser configuration, and it leads to a minimum energy proportional to E_{Rec}. The function f and the minimum kinetic energies were determined in 1D [10] and in 2D [11].

In this Letter we report on quantum calculations performed in 3D laser cooling. The conventional starting point for such a calculation is the master equation for the atomic density matrix ρ, representing the quantum states of the electronic and center-of-mass degrees of freedom. The number of elements of ρ is proportional to the square of the number of points in a grid covering the center-of-mass momentum range. For example, for $|p_i| \leq 20\hbar k$, $i = x, y, z$, and a discretization of $\hbar k$ we get $(2 \times 20 + 1)^6 \simeq 5 \times 10^9$ elements, a number which should be multiplied by the number of matrix elements relative to the atomic electronic states. A direct integration, like the one in 2D [12] can therefore not be performed. A reduction to rate equations for the diagonal elements of ρ in a proper basis was applied in 1D and 2D [10,11]. In 3D the condition for this approximation is not fulfilled for typical experimental parameters.

With this type of problem in mind we have recently developed a general formulation of dissipative problems in quantum optics replacing the density matrix by stochastic wave functions [13–15]. Inspired by other problems in quantum mechanics and quantum optics, other authors have developed similar formulations [16–19].

We now outline our application of this method to 3D laser cooling. The time evolution of a single stochastic wave function is characterized by intervals of Hamiltonian evolution interrupted by random quantum jumps accounting for the spontaneous emission of photons. We introduce the ground and excited state components of the atomic state vector $|\psi_g\rangle$ and $|\psi_e\rangle$, obeying the coupled linear equations

$$i\hbar \frac{d}{dt}|\psi_e\rangle = \left(\frac{\vec{p}^2}{2M} - \hbar\delta - i\hbar\Gamma/2\right)|\psi_e\rangle + V^{(+)}|\psi_g\rangle, \tag{2}$$

$$i\hbar \frac{d}{dt}|\psi_g\rangle = \frac{\vec{p}^2}{2M}|\psi_g\rangle + V^{(-)}|\psi_e\rangle. \tag{3}$$

Here, $\vec{p}$ denotes the atomic momentum operator, and Γ enters explicitly as a damping term in the evolution of $|\psi_e\rangle$. Equations (2) and (3) are obtained in a rotating frame where the atom-laser interaction is written in the rotating wave approximation as $V = -\vec{D}^{(+)} \cdot \vec{E}_L^{(+)} +$ H.c., with $\vec{D}^{(+)}$ being the raising part of the atomic dipole operator and $\vec{E}_L^{(+)}$ the amplitude of the positive frequency component of the laser electric field.

The state vector also undergoes quantum jumps at instants chosen according to the current spontaneous

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emission rate $dP/dt = \Gamma\langle\psi_e|\psi_e\rangle/\langle\psi|\psi\rangle$. The emission of a photon with a polarization $\vec{\varepsilon}_S$ and a wave vector $\vec{k}_S$ corresponds to a change of the state vector

$$|\psi\rangle \longrightarrow |\psi\rangle_{\vec{k}_S,\vec{\varepsilon}_S} = (\vec{\varepsilon}_S^{\,*} \cdot \vec{D}^{(-)}) e^{-i\vec{k}_S\cdot\vec{R}}|\psi_e\rangle, \qquad (4)$$

and it has a relative probability $\||\psi\rangle_{\vec{k}_S,\vec{\varepsilon}_S}\|^2$. The exponential factor containing the position operator $\vec{R}$ of the atom translates the atomic momentum by the recoil momentum $-\hbar\vec{k}_S$, the operator $\vec{\varepsilon}_S^{\,*} \cdot \vec{D}^{(-)}$ projects the atom onto the ground state, and the evolution proceeds from here according to Eqs. (2) and (3). Although the calculations can be performed with the exact dipole pattern for spontaneous emission [14], we have simplified to emission of photons along the coordinate directions $\vec{e}_x$, $\vec{e}_y$, and $\vec{e}_z$, only. This is justified by the widths of the calculated distributions being several $\hbar k$.

To identify the optimum laser cooling we shall use the fact [1,2] that polarization gradient cooling is most efficient at low saturation $s \ll 1$, to adiabatically eliminate the excited state. Neglecting $\vec{p}^2/2M$ as compared to $\hbar\Gamma/2$ and putting $d|\psi_e\rangle/dt = 0$ in Eq. (2), we obtain $|\psi_e\rangle = (\hbar\delta + i\hbar\Gamma/2)^{-1}V^{(+)}|\psi_g\rangle$. When inserted into Eq. (3), this introduces the effective ground state potential operator $(\hbar\delta + i\hbar\Gamma/2)^{-1}V^{(-)}V^{(+)}$. Since V is proportional to $\hbar\Omega$, we have, in this way, made appear frequencies $\sim|\delta|s$ (light shifts) and damping rates $\sim\Gamma s$ (optical pumping rates), which we require to be much smaller than Γ for consistency with the elimination of $|\psi_e\rangle$. This procedure removes the short times $1/\delta$ and $1/\Gamma$, so that time steps, longer by a factor $\sim 1/s$, may be applied in the integration of Eq. (3).

We now take the laser configuration to be a superposition of fields propagating along the coordinate axes. We expand the center-of-mass components of the wave function on a set of states with momenta $\vec{p} = \vec{p}_0(t) + \hbar k(n_x, n_y, n_z)$, where n_x, n_y, and n_z are integers. Indeed, an initial momentum eigenstate will, at any later times, have an exact expansion on these states, and with the simplified emission pattern described above, $\vec{p}_0(t)$ can be set to 0 at all times. In practice, we have to limit the momentum grid, and we consider it sufficient to take $-20 \le n_x, n_y, n_z \le 20$ for calculations of momentum distributions with $p_{i,\mathrm{rms}} \le 7\hbar k$, $i = x, y, z$, the maximum considered in this paper.

The integration of Eq. (3) with $|\psi_e\rangle = (\hbar\delta + i\hbar\Gamma/2)^{-1}V^{(+)}|\psi_g\rangle$ follows a splitting technique. To obtain the wave function $|\psi_g(t + dt)\rangle$ from the value at time t, we first multiply components of momentum $\vec{p}$ by the kinetic energy phase factor $\exp(-i\vec{p}^2 dt/2M\hbar)$. Second, we approximate the propagation due to V by a fourth order Taylor expansion in powers of dt, requiring $|\delta|sdt < 1$. The first neglected terms due to the splitting are proportional to $[\vec{p}^2/2M, V^{(-)}V^{(+)}/(\hbar\delta + i\hbar\Gamma/2)](dt/\hbar)^2 \sim (kpdt/M)|\delta|sdt$, and this puts an additional criterion on the maximum allowable time step dt. In our calculations we applied a time step of $dt = 0.025(\Gamma s)^{-1}$.

The Monte Carlo wave-function method is a simulation technique, and the restriction to a finite number of state vectors leads to error bars on our results. Suppose that at time t, n independent wave functions $|\psi_i(t)\rangle$ have been evolved, and that the expectation values $a_i(t) = \langle\psi_i|A|\psi_i\rangle/\langle\psi_i|\psi_i\rangle$ of an atomic operator A have been calculated for the n wave functions. The sample mean of the a_i's, $\langle a\rangle = (\sum_{i=1}^{n} a_i)/n$, then gives an approximation to the exact mean value, $\mathrm{Tr}[\rho(t)A]$, with a statistical error estimated by $\delta a/\sqrt{n}$, where $(\delta a)^2$ is the sample variance of the a_i's [14]. The statistical error will therefore be represented in our figures by error bars with a half-width $\delta a/\sqrt{n}$.

Here, the atomic density matrix $\rho(t)$ converges to a steady state ρ^{st} within a time τ of order the relaxation time of the mean kinetic energy. In the Monte Carlo simulation, the wave functions have no steady state, so that each expectation value $a_i(t)$ keeps fluctuating with time. In the derivation of steady-state mean values, one may, however, replace the variables $a_i(t)$ by their time average $\bar{a}_i$ on a time interval $\gg\tau$. An approximation of $\mathrm{Tr}(\rho^{\mathrm{st}}A)$ is then derived from the sample mean of the $\bar{a}_i$'s, with a statistical error $\delta\bar{a}/\sqrt{n}$, where $(\delta\bar{a})^2$ is the sample variance of the $\bar{a}_i$'s. For the interaction times considered, this time averaging procedure leads to $\delta\bar{a} \sim \delta a/3$, for $A = \vec{p}^2$, mimicking an increase in the number of wave functions by a factor of 9.

Measurements of temperatures in 3D optical molasses have been performed on $j_g \rightarrow j_e = j_g + 1$ atomic transitions, with $j_g = 2$ and $j_g = 3$ in two isotopes of Rb [2] and with $j_g = 4$ in Cs [1]. We present results for these three types of transitions, and for $j_g = 1$. Also, we restrict ourselves to one closely investigated laser configuration, the so-called lin $\perp$ lin configuration, defined by the electric field

$$\vec{E}_L^{(+)}(\vec{r}) = \frac{E_0}{2}[e^{i\phi_x}(\vec{e}_y e^{ikx} + \vec{e}_z e^{-ikx}) + e^{i\phi_y}(\vec{e}_z e^{iky} + \vec{e}_x e^{-iky}) + e^{i\phi_z}(\vec{e}_x e^{ikz} + \vec{e}_y e^{-ikz})]. \qquad (5)$$

The amplitude E_0 is included in the Rabi frequency $\Omega = dE_0/\hbar$, where d is the atomic dipole moment.

In Fig. 1 the mean steady-state kinetic energy of the atoms E_K is shown as a function of the parameter $\hbar|\delta|s/2$, for laser phases $(0, 0, 0)$ and a detuning of $\delta = -5\Gamma$. We recover the characteristic functional dependence of E_K described in the introduction. For a large light shift, $E_K \simeq a\hbar|\delta|s/2 + bE_{\mathrm{Rec}}$. For decreasing values of the light shift, E_K goes through a minimum and then increases sharply, indicating the existence of a threshold for polarization gradient cooling to be effective. We note the dependence of E_K on the angular momentum j_g, the largest values of j_g giving rise to the coldest atomic distributions. The slope a and the minimum mean kinetic energy are given in Table I, as functions of j_g, together with experimental values for $j_g > 1$. The number of Monte Carlo wave functions ranges from 6

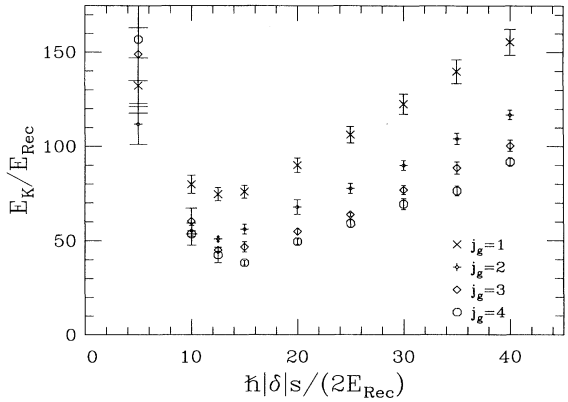

FIG. 1. Mean kinetic energy as a function of light shift for the atomic transitions $j_g \rightarrow j_e = j_g + 1$, $j_g = 1, 2, 3$, and 4. The laser field configuration is given by (5) with $\phi_x = \phi_y = \phi_z = 0$, and the atom-laser detuning is $\delta = -5\Gamma$.

to 12. In the affine regime, the points were obtained with an interaction time of $400(\Gamma s)^{-1}$, with the temporal average performed over the last $200(\Gamma s)^{-1}$, whereas close to threshold, relaxation times get longer and interaction times up to $800(\Gamma s)^{-1}$ were considered. The calculation per point required the equivalent of 10 to 50 h on a Cray C90 computer. In the experiments quoted above, the phases of the six laser beams were not controlled. In order to validate our comparison with the measurements we have extended our $j_g = 2$ calculations to the phase $(0, \pi/3, 2\pi/3)$. Within our error bars the minimum kinetic energy and the slopes are the same as in Fig. 1.

The Monte Carlo wave functions provide much more information than shown in Fig. 1. An aspect of laser cooling which has received much interest [20,21] is the possibility to form spatially periodic atomic distributions. In Figs. 2(a) and 2(b) we show position distributions calculated for two different sets of phases. We interpret the observed localization in terms of the spatial variation of the laser fields. In the case of vanishing phases, the electric field on the line $x = y = z$ is linearly polarized. The maximum intensity is obtained on this line at $(x, y, z) = (0, 0, 0)$ and at $(\lambda/2, \lambda/2, \lambda/2)$. But, because circularly polarized light interacts more strongly with $j_g > 0 \rightarrow j_e = j_g + 1$ transitions (Clebsch-Gordan coefficients), it may be advantageous for the atoms to localize at a distance from this line, where a larger fraction of circularly polarized light is present. This qualitatively explains the doughnut-shaped distributions shown in Fig. 2(a), a shape also obtained in semiclassical calculations [7]. The

TABLE I. Results of Fig. 1 ("calc," vanishing phases) and experimental results ("meas," uncontrolled phases) for the minimum kinetic energy and for the slope a (see text).

j_g	E_K^m/E_{Rec}(calc)	E_K^m/E_{Rec}(meas)	a(calc)	a(meas)
1	74.7 ± 3.5	···	3.3 ± 0.5	···
2	51.0 ± 1.4	50 ± 5	2.6 ± 0.2	2.3 ± 0.2
3	45.1 ± 1.1	50 ± 5	2.5 ± 0.2	2.1 ± 0.2
4	38.3 ± 1.2	40 ± 10	2.1 ± 0.2	2.1 ± 0.5

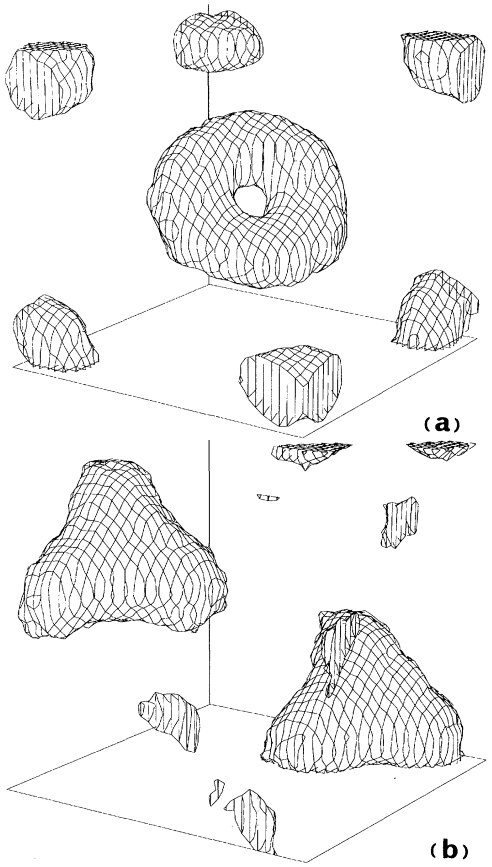

FIG. 2. Atomic position distributions in the cell $-\lambda/2 < x, y, z < \lambda/2$, for a $j_g = 2 \rightarrow j_e = 3$ transition, with $\hbar|\delta|s/2E_{Rec} = 30$ and $\delta = -5\Gamma$. The probability of finding the atom within the surfaces of constant density shown is 1/4. The corresponding enclosed volume is 6% for (a) (vanishing phases) and 8% for (b) [phases $(0, \pi/3, 2\pi/3)$].

situation for the case of $(\phi_x, \phi_y, \phi_z) = (0, \pi/3, 2\pi/3)$ is completely different. Now, the maximum intensity is obtained in the points $(x, y, z) = (\lambda/6, 2\lambda/3, \lambda/6)$ and $(2\lambda/3, \lambda/6, 2\lambda/3)$, where the light is circularly polarized. It follows that the optically induced potential wells have absolute minima here and, indeed, atoms are localized around these points; see Fig. [2(b)].

Also, fast atoms may localize within the plane perpendicular to their velocity. For example, for the set of phases $(0, \pi/3, 2\pi/3)$ we have identified lines through the points of maximum intensity and with direction $(1, 1, 1)$, where the light has a constant circular polarization [orthogonal to $(1, 1, 1)$], and where the localization of atoms with high velocities along $(1, 1, 1)$ is likely to occur. As the polarization is constant here we expect a less efficient cooling of these atoms and therefore an anisotropy in the momentum distribution. In a two-dimensional optical lattice this anisotropy leads to escape channels for the atoms for sufficiently small light shifts $\hbar|\delta|s$ [12].

Below the value of light shifts leading to the minimum kinetic energy we get a momentum distribution as exem-

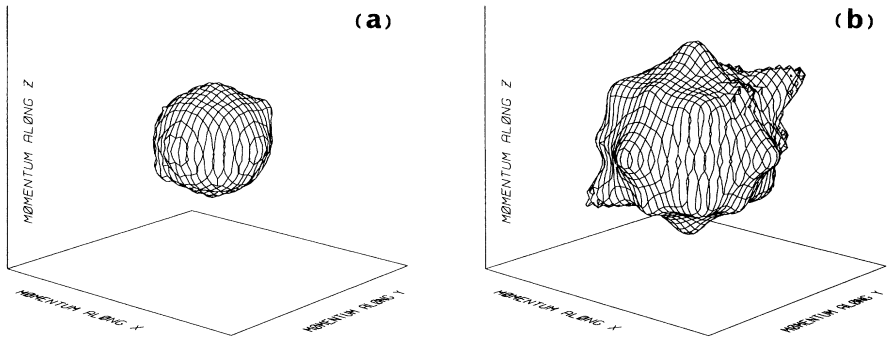

FIG. 3. Momentum distribution for a $j_g = 2 \rightarrow j_e = 3$ transition, with $\hbar|\delta|s/2E_{\mathrm{Rec}} = 5$ and $\delta = -5\Gamma$, and for the phases $(0, \pi/3, 2\pi/3)$. The plotted isodensity surfaces correspond to 1/15 (a) and 1/50 (b) of the maximal density. Similar results are obtained for vanishing phases.

plified in Fig. 3. The central part of the distribution is essentially isotropic; in an intermediate range [Fig. 3(a)] we recover the expected anisotropy along $(1, 1, 1)$ giving rise to a lemon-shaped isodensity surface, and in the far wings [Fig. 3(b)] further escape lines are visible. In fact, escape lines may exist in all directions $\vec{n}$ with transverse cooling, i.e., orthogonal to two Fourier components $\vec{k}_a - \vec{k}_b$, $\vec{k}_{a'} - \vec{k}_{b'}$ of $V^{(-)}V^{(+)}$, the $\vec{k}$'s being wave vectors of the laser beams. The relative importance of the escape lines, however, is difficult to assess when they are not associated to constant circular polarization.

In conclusion, we have shown that the Monte Carlo wave-function method applies successfully to the problem of 3D laser cooling. Mean kinetic energies in good agreement with the experimental values have been obtained, and we have discussed features of the cooled distributions which have not yet been measured. The low level of statistical uncertainty on our results was beyond our expectations and strongly relies on the time averaging procedure. This brings promises for further applications within this field, and we are currently investigating nonperiodic problems, appearing in connection with spatial diffusion and neutral atom traps.

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