Cold collisions between atoms in optical lattices

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We have simulated binary collisions between atoms in optical lattices during Sisyphus cooling. Our Monte Carlo Wave Function simulations show that the collisions selectively accelerate mainly the hotter atoms in the thermal ensemble, and thus affect the steady state which one would normally expect to reach in Sisyphus cooling without collisions.

Neutral atoms can be cooled and trapped in light-induced optical lattices [1]. By controlling the laser light one can adjust the properties of the lattices in order to study e.g. the quantum nature of atomic motion in a periodic structure [2], including the analogues to the behavior of electrons in periodic solid state lattices [3]. Ideas regarding the possibility to use optical lattices in atom optics and quantum computation have also emerged recently [4–7]. In experiments the trapped gas density is typically very low, providing for the moment at best a filling ratio of 10% for the near red detuned lattices [1]. Thus it is a priori a good approximation to ignore that the atoms interact with each other. In magneto-optical traps for cold atoms the inelastic collisions limit the numbers and temperatures achievable for the atomic gas as densities increase to about 10^11 atoms/cm^3 [8]. By using Bose-Einstein condensates or combining lattices and other types of optical traps it is becoming possible to obtain filling ratios close to unity and even higher [1]. We have considered mainly the case where the filling ratio is about 25%, but our results can be qualitatively interpolated for smaller ratios. Applications such as quantum computing require atoms to interact in order to perform quantum logical operations [1,4,8].

Controlled interaction studies in optical lattices could be performed e.g. by superimposing two optical lattices, which can be moved in respect to each other [9]. This, however, does not answer the question of what happens in a basic lattice configuration when the filling ratio increases, especially when inelastic collisions interfere with the cooling process and localization of atoms at lattice sites. For low densities the atom cloud reaches a thermal equilibrium state, and based on the studies in magneto-optical traps one would expect that inelastic collisions increase the temperature of this equilibrium state as the gas density increases [10]. We have performed Monte Carlo Wave Function (MCWF) simulations of two atoms in a lattice. They show that (for the parameters of our study) an equilibrium is not easily obtained. Instead, the hotter atoms are selectively accelerated, and, especially in 2D lattices, are likely to leave the lattice. Thus in densely populated lattices Sisyphus cooling could be assisted by an evaporation process: interactions eject the hotter atoms whereas the remaining atoms thermalize via Sisyphus cooling (in contrast to the collisional thermalization in evaporative cooling in magnetic traps).

In a collision two cold atoms get close enough to form a long-range quasimolecule [9]. Compared to single atoms, the quasimolecule interacts differently with the surrounding laser light, and this interaction depends on the interatomic distance. Previously the atomic interactions in lattices have been modelled by assuming fixed positions for both atoms and calculating how the atomic energy levels are shifted by the interaction [1,4]. Such static models ignore the dynamical nature of the inelastic collisions. But to allow the atoms to move makes the problem complicated and computationally tedious. We present in this Rapid Communication a study of collisions in a lattice between moving atoms. Once the dynamical processes are understood, they can be used as input for macroscopic theories. This approach leaves out many other aspects of the problem, such as reabsorption of scattered photons, which is another mechanism that strongly limits the densities in magneto-optical traps. Thus our results do not necessarily reflect the complete situation in optical lattices, but we believe they demonstrate the effect of collisions on Sisyphus cooling.

The distribution of atoms in an optical lattice depends on the choice of laser field configuration and the atomic level structure. The laser field should have a spatially changing polarization, and the atom needs at least two Zeeman sublevels in the lower energy state, and a different angular momentum in the upper energy state. The interaction between the laser field and an atom gives rise to periodic light-induced potentials for atoms in the Zeeman states of their internal ground states. A single atom moving in such a lattice will undergo Sisyphus cooling because of optical pumping from one ground state to another, in a manner that favors the reduction of kinetic energy between the rapid optical pumping cycles [5].
This cooling effect takes place rapidly in lattices created by lasers which are tuned only a few linewidths below the atomic transition. After cooling, the atoms are to a large extent localized in these potential wells.

We have chosen as a basis for our studies the simplest atomic transition for a red-detuned laser field, i.e., a system with a lower state angular momentum $J_g = 1/2$ and an upper state angular momentum $J_e = 3/2$. We denote the first state as the ground state and the second state as the excited state, with eigenstates $|e_{\pm 3/2}\rangle$ and $|e_{\pm 1/2}\rangle$. The resonance frequency of the transition is $\omega_0$. In the numerical calculations we have used the atomic properties of Cs.

The laser field has periodicity in one dimension, and consists of two linearly polarized counter-propagating beams, with orthogonal linear polarization and frequency $\omega$. For this configuration, the combined laser field is

$$E(z,t) = E_0(e^{ikz} - ie^{-ikz})e^{-i\omega t} + c.c.,$$

where $E_0$ is the amplitude and $k$ is the wavenumber.

When the interactions become important, the atomic cloud is still relatively dilute so that only two atoms at a time are involved, and the dipole-dipole interaction (DDI) dominates the process. We calculate the two-atom DDI potentials following the procedure described in Appendix A of Ref. [16]. We consider two atoms interacting with the laser field, coupled to a reservoir, namely the vacuum electric field. The system Hamiltonian reads (after rotating wave approximation)

$$H_s = \sum_{\alpha=1,2} \frac{\not{p}_\alpha^2}{2M} - \hbar \delta P_{e,\alpha} + V,$$

where the sum over $\alpha$ is over the two atoms, $\delta$ is the detuning $= \omega - \omega_0$, $M = 133$ a.u. is the Cs atom mass, and $P_{e,\alpha} = \sum_{m=\pm 3/2} |e_m\rangle_\alpha \langle e_m|$. The potential $V$ gives the interaction with the laser field. The strength of this interaction is given by the Rabi frequency $\Omega = 2dE_0/\hbar$ where $d$ is the dipole moment of the transition.

The system interacts with the reservoir through a dipole coupling between the atoms and the vacuum modes. As we want an expression for the DDI potential, we concentrate our effort on the calculations leading to an expression like Eq. (25) of Ref. [16], which originates from the commutator between the system density operator, $\rho$, and the DDI potential, $V_{dd}$. Also, we concentrate on spontaneous terms, i.e., terms with vanishing average photon number. Let us introduce the operators

$$S_{+q}^\alpha = \sum_{m=\pm 1/2} CG_{m}^q \langle e_{m+q} \rangle_\alpha \langle e_m|,$$

where $CG_{m}^q$ are the appropriate Clebsch-Gordan coefficients and $q$ is the polarization label in spherical basis. Furthermore, we use a description in terms of a center of mass coordinate $Z$ and a relative coordinate $r = r_2 - r_1$ (with coordinate along the quantization axis $z = z_2 - z_1$). With these coordinates, the interaction potential with the laser field reads

$$V = -i\frac{\hbar \Omega}{\sqrt{2}} \sin kZ \cos kZ \frac{S_{+q}^\alpha + iS_{-q}^\alpha}{2} + \hbar \Omega \cos kZ \frac{S_{+q}^\alpha + iS_{-q}^\alpha}{2} + \hbar \Omega \sin kZ \frac{S_{+q}^\alpha + iS_{-q}^\alpha}{2} + h.c.,$$

where $S_{+q}^\alpha = S_{+q}^1 + S_{+q}^2$ and $\Delta S_{+q} = S_{+q}^1 - S_{+q}^2$.

In order to calculate the DDI term, we look at the Hamiltonian part of the damping terms in the equation of motion for the system density operator $\rho$. After manipulations similar to those presented in Appendix A of Ref. [16] and using arguments from Ref. [17] to evaluate integrals of Bessel functions multiplied with principal value functions, we find the DDI potentials between the two atoms. In the following we look only at atoms on the axis of the laser field, i.e., a one-dimensional situation, and in this case, the DDI potential reduces to

$$V_{dd}^{axis} = \frac{3}{8} \hbar \Gamma \left\{ \frac{1}{3} \frac{\sin q_0 r}{(q_0 r)^2} + 2 \frac{\sin q_0 r}{(q_0 r)^2} \right\} \times (S_{+q}^1 S_{-q}^2 + S_{+q}^2 S_{-q}^1 - 2S_{+0}^1 S_{-0}^1).$$

Here, $\Gamma$ is the atomic linewidth, $q_0$ is the resonant wavenumber $q_0 = \omega_0/\epsilon$, and

$$S_{+q} S_{-q'} = (S_{+q}^1 S_{-q'}^2 + S_{+q}^2 S_{-q'}^1).$$

Numerical simulation of the motion of atoms in the lattice field in one dimension only, using the MCWF method [18], is computationally very demanding [19]. In order to perform two-atom studies, which require even in one dimension at least two translational degrees of freedom, we have fixed one atom in position, and let the other one move freely. This fixes the relation between the lattice coordinates and the relative interatomic coordinate. Thus an inelastic collision will not change the kinetic energy for both atoms, but we use the relative kinetic energy as an estimate for the kinetic energy change per atom. (We express energy and momentum in recoil units: $E_r = \hbar^2 k^2/2M$ and $p_r = \hbar k$ respectively).

We have formulated the problem in the two-atom basis, which leads to a system of 36 internal states. In studies for magneto-optical traps one tends to use the molecular frame, where the atom-atom interactions have been included to the molecular potential structure [21]. However, the quantum jump processes needed for the Monte Carlo method are easier to describe in the atomic basis. One aspect of the simulations is that we do not use the adiabatic elimination of the excited states [21], which is typically employed in order to simplify the equations for
atomic motion. For simplicity we neglect Doppler cooling (as Sisyphus cooling takes us below the Doppler limit, we expect it to be the dominant process). In the molecular frame the system of two interacting atoms is excited resonantly to a molecular state with an attractive interatomic potential \( \Phi \). This leads to the acceleration of the relative motion of the atoms, until the process terminates with spontaneous decay. We use these attractive potentials for the verbal description of the process but it must be emphasised that they do not directly appear in the two-atom basis. The kinetic energy change due to the attractive potentials also complicates greatly the numerical simulations by demanding larger momentum and finer spatial grid than in the single atom Sisyphus cooling simulations \([22]\).

We use the laser parameters \( \delta = -3\Gamma \) and \( \Omega = 1.5\Gamma \), which give a lattice modulation depth of \( U_0 = 584E_r \). These parameters correspond to a lattice where the atoms move from one lattice site to another on a timescale that is comparable to the timescale of a harmonic oscillation within one of the lattice potential wells. In our selected system the atomic interactions are too weak to really destroy the lattice, so the actual case of interest is the one where the atoms need to be simultaneously at the same lattice site.

In the MCWF method an approximation for the two-atom steady state density matrix is obtained as an ensemble average of different wave function histories, for which the spontaneous emission occurs as probabilistic quantum jumps \([18]\). These quantum jumps (both atoms in our case have six decay channels) occur according to probabilities weighted by the appropriate Clebsch-Gordan coefficients of the decay channels. There are various ways how to calculate the results by ensemble averaging. We take the ensemble average of single history time averages in the steady state time domain \([23]\). Thus we obtain the kinetic energy per atom, and the spatial and momentum probability distributions for various filling ratios \( \rho_o \) of the lattice.

A comparison between the number of atoms having gained large kinetic energy via interactions and the total number of interaction processes show (see Table \( \PageIndex{1} \)) that basically every collision produces very hot atoms in our chosen parameter range. This leads to evaporation in the optical lattice: those atoms which are able to move from one well to the other and which have larger kinetic energy than localized atoms leave the trap. A crucial ingredient in the interaction process increasing the kinetic energy by a large amount and leading to evaporation is that a large fraction of the population has to enter the attractive molecular excited state during the interaction process. This fraction in turn depends on the relative velocity between the interacting atoms when they reach the resonance point for the attractive molecular states. The relative velocity in turn depends on the lattice depth. In our simulations the surroundings is still favorable so that the relative velocity between atoms is low enough to keep the excitation probability high when atoms approach each other and cross the molecular resonance point.

The number of attractive molecular states is five and the resonant excitation to these potentials takes place at different interatomic distances \([20]\). If the atoms do not get a large increase in kinetic energy at the first resonance they reach, there are still other resonances left. A comparison with semiclassical (SC) excitation and survival calculations suggests that the potential which becomes resonant first when the atoms approach each other has the dominant role in the inelastic collision process.

When calculating the steady state kinetic energy per atom (Table \( \PageIndex{1} \)), we use two critical wavevectors \( k_c \). Wavefunction histories which at some time point have gained larger total kinetic energy than given by \( k_c \) are neglected in ensemble averaging (considered lost from the lattice). The smallest value of \( k_c \) we use \([22]\) is more than two times larger than the semiclassical critical value \( k_c^{sc} \) given in Ref. \([15]\). The denser the lattice is initially, the larger is the number of interaction processes and the more effective is the evaporative cooling process. This can be seen in the results for kinetic energy per atom using \( k_c = 40 \) (see Table \( \PageIndex{1} \)). The kinetic energy decreases when the initial density of the lattice increases. Results with \( k_c = 70 \) include atoms that are lost from the lattice, and the value of the kinetic energy is slightly above the sparse lattice (non-interacting case) result.

The momentum distribution in Fig. \( \PageIndex{1} \) shows the effect of the evaporative cooling process clearly. Due to the interactions between atoms part of the population has shifted to the region of large \( k \) (wings in Fig. \( \PageIndex{1} \)) and does not localize back to the lattice because the atoms are above the recapture range. Thus the central peak of the momentum distribution corresponding to atoms localized at lattice sites has a 13\% narrower FWHM for an initially dense lattice compared to the non-interacting case.

We have shown that in high-density, red-detuned (a few linewidths) optical lattices, atomic interactions could lead to the ejection of the hotter atoms from the lattice, or at least to a selective heating process accompanied by a narrowing of the central momentum distribution. This is because (a) atoms may move from one lattice site to another even in the steady state for Sisyphus cooling, and (b) because the molecular interaction is strong enough to give to each clearly interacting atom pair almost always enough energy to escape from the lattice. Earlier simulations for roughly the same laser (and Cs) parameters in magneto-optical traps indicate that the dominating effect is a clear broadening of the atomic momentum distribution, i.e., radiative heating \([14]\). In both situations high-momentum atoms are produced, but in optical lattices atoms with higher momentum are strongly favoured in the momentum increasing process (in both cases the fast atoms get involved in more close encounters than the
Due to the large kinetic energies, the spatial step size $\Delta z$ of the standard deviation for the kinetic energies are given in parentheses.

| $\rho_o(\%)$ | $N_{tot}^c$ | $N_{out}^c$ | $<E_k>$ | $<E_k>$ |
|-------------|------------|-------------|--------|--------|
| 25.0        | 39         | 38          | 26     | 61(6) 110(18) |
| 20.0        | 25         | 27          | 19     | 69(5) 99(12)  |
| 16.7        | 19         | 19          | 11     | 80(6) 103(12) |
| 14.3        | 16         | 19          | 12     | 80(7) 104(12) |

no interactions 0 0 0 91(8) 91(8)

has to be smaller than in single atom simulations since the momentum space size is $L_k = 2\pi/\Delta z$. We use the split operator Fourier method to solve the non-Hermitian time-dependent Schrödinger equation. The lattice density is controlled with the position space size $L_z$.

At the semiclassical value $k_c^sc$ the cooling force has its maximum value, but Sisyphus cooling is still effective above that point. Our values of $k_c$ gives a criterion for neglecting energetic histories from the ensemble (i.e., atoms lost from the lattice).

![FIG. 1. The steady state momentum probability distributions for a densely populated ($\rho_o = 25\%$) lattice and for the non-interacting atoms case (see text). All of the MC histories are included. Here $\delta = -3.0 \Gamma$, and $\Omega = 1.5 \Gamma$.](image-url)

TABLE I. Escaped atoms and kinetic energies. The number of MC histories which have been neglected ($N_{out}^c$) in the ensemble averaging due to escape from the lattice and steady state kinetic energies per atom ($<E_k>$) for various filling ratios ($\rho_o$) of the lattice. Two different critical wavenumbers $k_c$ have been used. $N_{tot}^c$ gives an estimate for the total number of atom-atom interaction processes based on single atom MC collision rate calculations by monitoring the quantum flux at a mean atomic separation given by $\rho_o$. The total number of MC histories for each simulation is 128. The absolute values of the standard deviation for the kinetic energies are given in parentheses.