Local dynamics of laser cooling in an optical lattice

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Using the basis of Wannier states, we study the local dynamics of polarization gradient cooling for an atom driven on a $J_g=2\rightarrow J_e=3$ transition by a one-dimensional optical lattice. This analysis allows us to formulate a physical picture of the cooling mechanism, analogous to Sisyphus cooling for a $J_g=1/2\rightarrow J_e=3/2$ atom, which depends strongly on coherences in the Zeeman sublevels of the ground state. In addition, we are able to explain the steady-state properties of the laser-cooled atoms in a regime where the standard semiclassical analysis breaks down. [S1050-2947(97)50309-X]

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The paradigm for sub-Doppler laser cooling is the Sisyphus effect as formulated by Dalibard and Cohen-Tannoudji [1]. The beauty of this model is that it gives a simple physical picture of the cooling mechanism. An atom driven on a $J_g=1/2\rightarrow J_e=3/2$ transition moves in a one-dimensional (1D) light field formed by two counterpropagating plane waves with orthogonal linear polarizations—the 1D lin\lin configuration. Cooling occurs as atoms are preferentially optically pumped from the peaks of the light shift potential associated with one ground state to the valleys of the other. Indeed, the simplicity of this model led to the realization of this 1D model in the laboratory, signifying a shift away from the image of atoms moving in a disordered “optical molas-" to that of an ordered “optical lattice” [2]. These experiments showed that in the steady state most of the atoms are trapped in the microscopic potential wells of the lattice, oscillating many periods before inelastic photon scattering occurs, and localized to a small fraction of the optical wave- length (the “oscillating regime”) [3].

Despite the considerable success of the simple Sisyphus model in explaining the basic steady-state properties of the laser-cooled atoms, there has been little detailed study of the dynamics. Recent experiments have shown some discrepancies with the dynamical model proposed in the simple Sisyphus picture [4]. The goal of this article is to develop a physical picture of the cooling mechanism applicable to the experiments: atoms with larger angular momentum trapped in the oscillating regime. Consider, for example, an atom with a ground-state angular momentum $J_g=2$ and excited state $J_e=3$, moving in a 1D lin\lin lattice. In this more complex system there is a set of optical potentials associated with the five ground states, coupled by stimulated Raman transitions. For such an atom, two possible semiclassical pictures of the cooling mechanism arise. In one [Fig. 1(a)], cooling occurs locally at a given lattice site as atoms preferentially climb steep potentials and descend shallow ones. Because of the difference in curvature between these two potentials, atoms expend more of their kinetic energy climbing wells than they regain on the descent, the difference being dissipated in optical pumping. Alternatively, atoms may cool when hopping between lattice sites by making nonadiabatic transitions between the coupled set of optical potentials and preferentially pumping to the potential with the largest light shift [Fig. 1(b)].

FIG. 1. Semiclassical pictures of Sisyphus cooling on a $J_g=2\rightarrow J_e=3$ transition. (a) “Local cooling” due to optical pumping within a given lattice site. (b) “Hopping cooling”: motional coupling causes transitions between the adiabatic potentials and atoms are optically pumped between lattice sites.
each with a corresponding Bloch wave function $u_{n,q,\xi}^{(m)}(z)$. The eigenvalue $\xi = \pm 1$ represents the symmetry of the wave function after a translation by $\lambda/4$, $u_{n,q,\xi}^{(m)}(z - \lambda/4) = \xi u_{n,q,\xi}^{(m)}(z)$ (the antiferromagnetic order of the linear lattice). Here we assume typical densities ($< 10^{12} \text{cm}^{-3}$) where atom-atom interactions, which would modify the lattice symmetries, can be neglected [11]. The Wannier spinor associated with the $n$th vibrational level at the $l$th lattice site is the Fourier transform of the Bloch spinor summed over all quasimomenta in the band,

$$|\Phi_{n,\eta}^{(l)}\rangle = \frac{1}{\sqrt{2N}} \sum_{n,q,\xi} |n,q,\eta,\xi\rangle (\xi e^{-i\eta/4})^{l} = \sum_{m_g,\eta} |\Phi_{n,m_g}^{(l)}\rangle \otimes |m_g\rangle. \quad (2)$$

Here $N$ is the number of full periods of the lattice to be included (each period contains two wells of opposite polarization), with the usual Born–von Karman periodic boundary conditions. As we are interested in the local cooling dynamics of nearly bound atoms we can employ a tight-binding approximation, and restrict our analysis to a lattice with only a few sites. Here we take a lattice extending from $-\lambda/2 < z \leq \lambda/2$, thus consisting of four wells, two $\sigma_+$ at $z = 0$, $\lambda/2 = \lambda/2$ and two $\sigma_-$ at $z = \lambda/4$, $-\lambda/4$. This includes tunneling effects over one wavelength. For two lattice periods, the quasimomenta are restricted to the center and edge of the Brillouin zone. In addition, for each quasimomentum there are two Bloch states associated with the antiferromagnetic order of the lattice, $\xi = \pm 1$, making a total of four Bloch states (four wells of the lattice).

We consider here an atom driven on a $J_z = 2 \rightarrow J_z = 3$ transition, moving in a 1D linear lattice; this is the smallest angular momentum for which the proposed local-cooling model is possible. Figure 2(a) shows the structure of the first six energy bands for $\eta = +1$ ($m_g = +2, -2$) with the diabatic well depth $U_0 = 200E_R$, where $E_R$ is the recoil energy. The Wannier wave functions at a $\sigma_+$ site associated with these bands are shown in Fig. 2(b). For strongly bound bands, the Wannier spinor is almost purely $m_g = +2$ ($99.8\%$ for $n = 0$), with wave functions very close to that of a simple harmonic oscillator. For excited bands there is more coherent mixing of the $m_g$ states as the atom samples more of the opposite polarization. There is a large jump in the amount of mixing for bands with energies above the $m_g = 0$ diabatic potential; e.g., for $n = 5$, the Wannier spinor is $43.9\%$ $m_g = +2$ and $47.0\%$ $m_g = 0$. Notice that the higher-lying wave functions are quite different from what one would calculate for the adiabatic potentials. This indicates that motional coupling is important for energies just slightly above or below the crossing points of the various optical potentials.

Given a basis describing the coherent coupling of an atom and the optical lattice, laser cooling is studied via the master equation [2],

$$\frac{d\rho}{dt} = \frac{1}{i\hbar} [H, \rho] - \frac{\gamma_s}{2} \sum_{\mu,h} N_{h,\mu} \times (W_{h,\mu}^{\dagger}W_{h,\mu}\rho + \rho W_{h,\mu}^{\dagger}W_{h,\mu} - 2 W_{h,\mu}\rho W_{h,\mu}^{\dagger}). \quad (3)$$

The relaxation part of the master equation is proportional to the photon scattering rate $\gamma_s$. The ‘jump operator’ $W_{h,\mu}$ represents absorption of a lattice photon followed by emission of a fluorescence photon with helicity $h$ into the direction $\mu = \cos \theta$ (relative to the $z$ axis), weighted by the probability distributions associated with the dipole pattern $N_{h,\mu}$. In general, spontaneous emission couples all quasimomenta within the first Brillouin zone. As we have restricted the lattice to only four wells, with the resulting restriction on quasimomenta, we take a simplified pattern for the spontaneous emission so that photons are either emitted along or perpendicular to the lattice axis.

The density operator is expanded in the basis of Wannier states as described above. We solve for the time-dependent populations in the rate equation approximation, setting all off-diagonal elements of the density operator to zero. Coherences between different vibrational levels can be neglected under the secular approximation when the energy spacing between the bands is large compared with the optical pumping rate out of the level [9]. Neglecting off-diagonal elements between Wannier states for the same vibrational level but at different lattice sites is appropriate when the tunneling rate between wells is small compared with the photon scattering rate, and when above-barrier ballistic motion is negligible. This approximation is valid for the bound bands in the Lamb-Dicke regime and for lattice parameters in the oscillating regime.

The rate equations in the Wannier basis take the form

$$\dot{\Pi}_{n,\eta}^{(l)} = \sum_{n',\eta',l'} \left[ -\gamma(n, \eta, l \rightarrow n', \eta', l)\Pi_{n,\eta}^{(l)} + \gamma(n', \eta', l' \rightarrow n, \eta, l)\Pi_{n',\eta'}^{(l')} \right], \quad (4)$$

where $\Pi_{n,\eta}^{(l)}$ is the population of the $n$th vibrational level at the $l$th lattice site for the family $\eta$ and...
is the transition rate between two Wannier states. The transition matrix element accounts for both the overlap of the internal degrees of freedoms (Clebsch-Gordan coefficients) and the external degrees of freedom (Franck-Condon factor). Calculation of these matrix elements is simplified through use of the symmetries of the lattice; a complete description of the resulting selection rules will be described elsewhere [12]. Steady-state solutions are easily obtained, and the full time-dependent solution can be computed for a sufficiently small number of vibrational levels. We find it necessary to retain a vibrational ladder up to an energy just above the $m_g=0$ diabatic potential; more levels change the steady-state population distribution by only a few percent. For a lattice with $U_0=200E_R$, we find that the steady-state populations in the first few vibrational levels of any given well are $\Pi_0=0.35, \Pi_1=0.23, \Pi_2=0.15$, and $\Pi_3=0.098$. By fitting the populations with a Maxwell-Boltzmann distribution we extract a temperature. Figure 3(a) shows the calculated temperature as a function of the light shift, exhibiting the usual linear dependence, $k_BT=0.22U_0$ (ignoring the intercept at $U_0=0$). Empirical results differ slightly [13]; this may be attributed to the different angular moments associated with the atomic transitions. In addition, we can extract the atomic localization as the population weighted sum of the localization of the Wannier states, automatically accounting for any anharmonicity in the potential. The localization is essentially independent of light shift, $\langle \Delta z \rangle = \lambda/14$, in general agreement with numerical simulations [14], and as measured in fluorescence [2] and Bragg scattering [4].

By choosing the basis of local Wannier states we can artificially "turn off" channels associated with local or hopping transitions and thereby identify the cooling mechanisms. Consider a lattice of "hot" atoms filling the lattice at $t=0$, so that all bound vibrational levels are occupied with equal probability. In the approximation that the populations remain in a Boltzmann distribution throughout the evolution, the ratio of the population of the first excited state to the ground state gives a measure of the temperature. This ratio is calculated as a function of time following four different sets of allowed transitions: (i) all possible transitions are retained between all the Wannier states, (ii) all "hopping transitions" (i.e. transitions between Wannier states associated with different wells) are set to zero, (iii) channels are set to zero in which the atom optically pumps from $m_g$ even to $m_g$ odd within the same well, i.e. no local cooling as in Fig. 1(a), and (iv) both local and hopping channels (ii)-(iii) are set to zero. The results are shown in Fig. 3(b). We see that the coldest temperature is achieved when all transitions are retained, $k_BT\approx 66E_R$ (in the harmonic approximation), or a steady-state ratio $r(\infty)=\Pi_1(\infty)/\Pi_0(\infty)=0.655$. Neglecting the hopping channels increases the steady-state ratio to $r(\infty)=0.80$, which doubles the temperature, whereas turning off the local channels (iii) leaves the ratio virtually unchanged, $r(\infty)=0.66$. By neglecting both hopping and local channels (ii) and (iii), there is very little cooling $r(\infty)=0.96$. Each of the time-dependent curves is fit to a single exponential of the form $r(t)=r(0)e^{-\gamma t}$, with the results $\alpha_{(i)}=0.038\gamma_s, \alpha_{(ii)}=0.022\gamma_s, \alpha_{(iii)}=0.037\gamma_s$, and $\alpha_{(iv)}=0.014\gamma_s$, where $\gamma_s$ is the photon scattering rate. Similar results hold for deeper potentials (e.g., $U_0=500E_R$) where there are even more possible channels for local cooling [12].

From these data we draw the following conclusions. Though there is some local cooling, the dominant mechanism is hopping cooling, with a rate nearly twice as large. This rate is in agreement with recent measurements, where the cooling time constant for a 1D lattice was found to be about 30 photon scatterings [4]. Though there is residual local cooling due to optical pumping within the same family of $m$ states (e.g., $m_g=0\rightarrow m_g=2$), the result of (iii) gives strong evidence that the local cooling mechanism depicted in Fig. 1(a) is negligible.

One can understand this cooling mechanism by looking directly at the transition rates between the Wannier states. We know that in the steady state the majority of the population is in the first few vibrational levels. How is this steady state maintained in a detailed balance? Heating of the bound states occurs due to spontaneous Raman scattering as atoms absorb and emit on the cycling transitions. Eventually this energy must be dissipated via optical pumping. If the atom is in a stretched state (e.g., $m_g=2$) and well localized near a site of $\sigma_+$ laser polarization, optical pumping is heavily suppressed due to a small Clebsch-Gordan coefficient (for $|j_{\uparrow}=2, m_g=2\rangle \rightarrow |j_{\uparrow}=3, m_g=1\rangle$, the coefficient squared is $1/15$). However, as the atom heats up the vibrational ladder it will reach an energy at which there is substantial coherent mixing of $m_g=2$ with $m_g=0$. Optical pumping is then very
probable from \( m_g = 0 \) to \( m_g = \pm 1 \), which has a deeper light shift, and from there the atom will optically pump back to the stretched state. Thus, coherent mixing of the \( m_g \) states provides the major channel for cooling.

The preceding addressed the internal degrees of freedom in the cooling transitions. The question of local vs hopping cooling depends on the overlap of the external degrees of freedom. For an atom starting in a \( \sigma_+ \) well, optical pumping from \( m_g = 0 \) to \( m_g = +1 \) or \( m_g = -1 \) is equally probable solely given the Clebsch-Gordan coefficients. The former would correspond to local cooling and the latter to hopping cooling. For the fifth vibration level in Fig. 2 (the major channel for cooling), the \( m_g = 0 \) Wannier wave function becomes delocalized, with most of its support in the neighboring well. Thus, this component of the atomic wave function will sample mostly \( \sigma_- \) radiation and pump into the \( m_g = -1 \) ground state of the neighboring well. Though the population in this high-lying vibrational level is small, the amount of energy dissipated in optical pumping is large, providing the detailed balanced necessary to maintain the steady-state temperature. From a semiclassical point of view, the atom is undergoing nonadiabatic transitions with respect to its internal degrees of freedom and follows a trajectory like that depicted in Fig. 1(b).

This mechanism also allows us to understand the steady-state properties of the laser-cooled atoms. The major channel for cooling occurs at an energy where there is substantial mixing of the \( m_g \) states. In our model this level occurs near the crossing point of the \( m_g = \pm 2 \) and \( m_g = 0 \) diabatic potentials. As the intensity of the lattice increases, the energy of this level increases linearly from the bottom of the well as measured in absolute units, but it is always the same fraction of the total light shift. Since atoms essentially fill the potential well up to this level, the steady-state atomic temperature will increase linearly with the depth of the potential, while the mean atomic localization within the well will be approximately intensity independent.

In conclusion, we have formulated a physical picture for the dynamics of laser cooling in optical lattices using a local basis of Wannier states. Such an analysis allows us to identify the major cooling channels and qualitatively understand the steady-state properties of the atoms. In the future, the development of the local Wannier basis may be useful for analyzing coherent quantum transport phenomena such as Bloch oscillations and Wannier-Stark spectroscopy [15].

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