Quantum-Mechanical Simulation of an Atomic Beam Focused by an Optical Standing Wave *

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(Received 3 December 2001)

Recent experiments have demonstrated that the light pressure force from an optical standing wave (SW) focuses an atomic beam to sub-micrometre dimensions. We start from a two-dimensional time-dependent Schrödinger equation and reduce it to a one-dimensional equation by a paraxial approximation. We calculate some theoretical limits on the focusing of an atomic beam by an SW optical field. It is found that two parameters, the atomic velocity and the intensity of the laser beam, play an important role in determining the deposition quality.

PACS: 03. 75. Be, 32. 80. Lg, 42. 82. Cr, 85. 40. Ux

The focusing of neutral atoms using near-resonant light fields has been an interesting subject recently. This has been stimulated to a large extent by the possibility of generating focal spots on the nanometre scale using specially configured laser intensity profiles. Particularly, it is interesting that the high-resolution focusing is combined with atomic deposition on to a substrate.[1,2] This technique has been termed atom lithography.[3] As a consequence of the small de Broglie wavelength, atom lithography has the potential for high resolution.[4]

The atom-lithography experiments have been performed with a particle optics approach and in terms of time-dependent classical trajectories of atoms. Some important factors that determine the outcome of the experiments have been identified and the experimental techniques have been progressively refined since the early demonstrations, resulting in significant improvements in both resolution and contrast. The classical analyses predict that one could obtain features as narrow as $5-10\,\mathrm{nm}$. Ultimately, the feature size should be limited by the wave nature of the atom, and it is interesting to discover what the limits are. Classical approaches can obtain only rough estimates.[5]

The light force on an atom has been studied widely.[6] In general, the force felt by an atom in a light field can be decomposed into both velocity-dependent and conservative terms. The velocity-dependent term, which arises from Doppler shifts experienced by the atom and from nonadiabatic effects, has been utilized extensively for laser cooling.[7] Many practical applications have made use of these dissipative terms, such as the slowing and trapping of atoms and the collimation of atom beams to a high degree. However, the velocity-dependent terms must be negligible if a particle-optical approach to the laser focusing of atoms is to be applicable in a straightforward way. Many of the fundamental concepts in particle optics presume a conservative potential.

Fortunately, for a wide range of parameters the velocity-dependent terms in the light force can be ignored, and a conservative potential can be derived. In this regime the light force is often referred to as the dipole force. If the laser intensity is relatively high and the detuning from the resonance is relatively small, the potential is[8]

$$U(x,y,z)=\frac{\hbar\Delta}{2}\ln\left[1+p(x,y,z)\right] \qquad (1)$$

with

$$p(x,y,z)=\frac{I(x,y,z)\gamma^2}{I_s(\gamma^2+4\Delta^2)}, \qquad (2)$$

where γ is the natural linewidth of the atomic transition, Δ is the detuning of the laser frequency of the atomic resonance, $I(x,y,z)$ is the laser intensity, and I_s is the saturation intensity associated with the atomic transition.

In this Letter, we have ignored any y-dependence of the laser intensity because it is assumed that any light force along this direction will be negligible compared with that from the standing wave.[9] We assume that the optical potential for the focusing experiment has the form of

$$U(x,z)=U(x)g(z), \qquad (3)$$

where the envelope function $g(z)$ is the profile of the laser beam along the z-direction, e.g. a Gaussian.[9] $U(x)$ is the conservative pseudopotential[10]

$$\begin{aligned}U(x)&=\frac{\hbar\Delta}{2}\ln\left[1+p(x)\right]\\&=\frac{\hbar\Delta}{2}\ln\left[1+\frac{p_0}{2+p_0}\cos(2kx)\right],\end{aligned} \qquad (4)$$

where $k=2\pi/\lambda$ is the wave vector of the laser light, $p_0=p/\cos(kx)^2$. For $\Delta<0$ we expand Eq. (4) to second order about $x=0$. Throwing out the constant terms, we find that the optical potential along the x-axis is a parabolic potential

$$U(x)\approx\frac{k^2\hbar\Delta p_0}{2(1+p_0)}x^2. \qquad (5)$$

*Supported by the Innovation Project Foundation of the Chinese Academy of Sciences under Grant No KJCX2-W7, and the National Natural Science Foundation of China No 10074072.

The two-dimensional time-dependent Schrödinger equation is then

$$H\Psi(x,z,t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(x,z,t), \tag{6}$$

where the Hamiltonian is

$$H = H_0 + U = -\frac{\hbar^2}{2m}\nabla^2 + U(x,z) \tag{7}$$

with m being the mass of atoms.

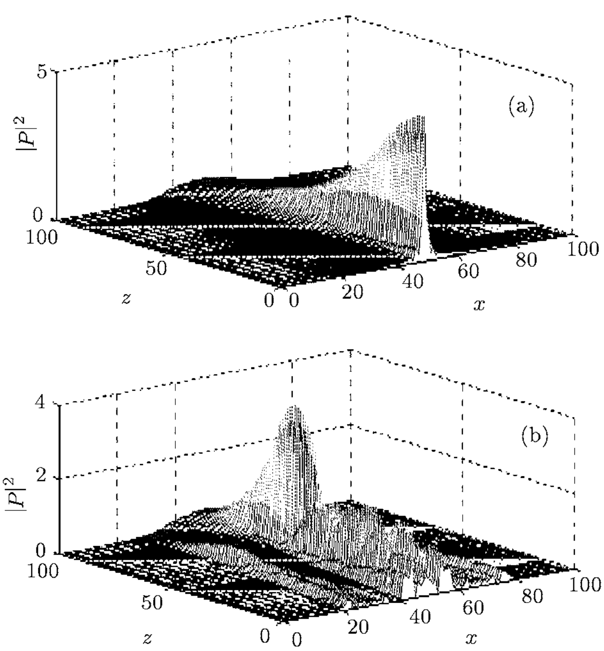

Fig. 1. Atom wave packet through the potential as described by Eq. (6) for the propagation distances of (a) 78 and (b) 140 (in units of laser beam radius) with a laser intensity of $20\,\mathrm{mW/cm^2}$ in the region $-\lambda/4 \le x \le 3/4\lambda$.

We choose the initial wave packet to be a Gaussian in the z- and x-directions,[11] propagating as a plane wave with momentum $\hbar k_{z_0}$ along the z-direction

$$\begin{aligned}\psi(x,z,0) &= \psi_1(x,0)\psi_2(z,0)\\ &= \frac{1}{\sqrt[4]{2\pi\sigma_x^2}}\exp(-\frac{x^2}{4\sigma_x^2})\frac{1}{\sqrt[4]{2\pi\sigma_z^2}}\\ &\quad\cdot\exp(-\frac{z^2}{4\sigma_z^2})\exp(\mathrm{i}k_{z_0}z),\end{aligned} \tag{8}$$

where the widths of these Gaussians are chosen to be $\sigma_z \gg \sigma_x$ and thus

$$\Psi(x,z,t) = \exp[-\mathrm{i}E(k_{z_0})\frac{t}{\hbar}]\psi(x,z,0). \tag{9}$$

Substituting Eq. (9) into Eq. (6) yields the stationary Schrödinger equation in two dimensions

$$\nabla^2\psi(x,z) + \frac{2m}{\hbar^2}\left[E(k_{z_0}) - U(x,z)\right]\psi(x,z) = 0. \tag{10}$$

By using a paraxial approximation, the spatial evolution of the atomic wavefunction $\Psi(x,z)$ along the z-direction is then described by the Schrödinger equation[9,11]

$$\mathrm{i}\hbar\nu_0\frac{\partial}{\partial z}\Psi(x,z) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x,z)\right)\Psi(x,z), \tag{11}$$

where ν_0 is the centre-of-mass velocity of the incoming atoms in the z-direction. The presence of the optical potential $U(x,z)$ can be treated as a small perturbation to the propagation of the wave packet along the z-direction.

Equation (11) is a parabolic partial differential equation that can be solved by different techniques. One convenient method is to use the finite-difference approximation via the ordinary differential equations. Using the algorithm in Ref. [11], we can solve the equation and evolve the wave packet through the two-dimensional region. The whole calculation is carried out in the range of one wavelength, $-\lambda/4 \le x \le 3/4\lambda$, and the output is the square of the wavefunction $|P|^2$.

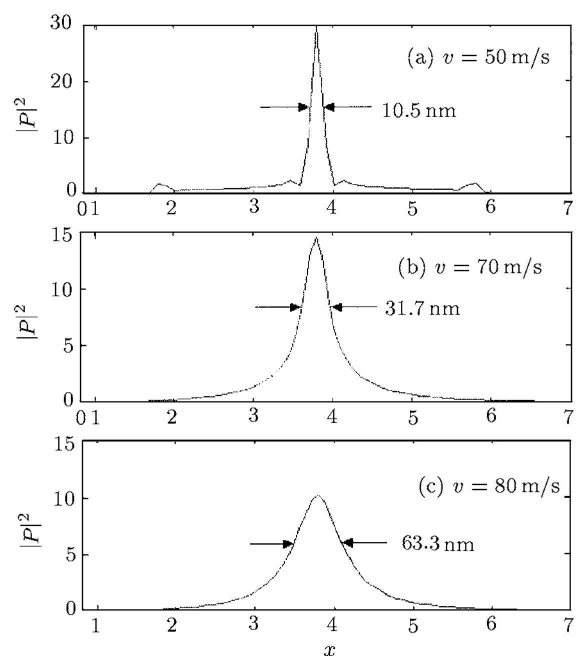

Fig. 2. Probability distribution of the atom wave packet at the same travel distance along the z-axis ($L = 78$, in units of laser beam radius) with the same optical intensity ($I = 20\,\mathrm{mW/cm^2}$) in the region $-\lambda/4 \le x \le 3/4\lambda$, for various initial velocities.

As an example, we consider a thermal Rb beam with an initial velocity from $v = 20\,\mathrm{m/s}$ to $130\,\mathrm{m/s}$, $\Omega_{\max} = 100\,\mathrm{MHz}$, and $\Delta = 100\,\mathrm{MHz}$. ($\Omega_{\max}$ denotes the Rabi frequency at the field antinode.) The laser beam radius is chosen as $r = 0.1\,\mathrm{cm}$. For these parameters, the laser intensity is selected from $5.0\times10^{-4}\,\mathrm{W/cm^2}$ to $5.0\times10^{-1}\,\mathrm{W/cm^2}$. The width of the initial atomic wave packet is chosen to be $\delta_z = 1$ (in units of laser beam radius) and $\delta_x = 4$ (in units of laser wavelength 780 nm). We do not consider the effect of the transverse velocity of the atomic beam, so the input parameters of the atomic velocity are all chosen along the z-direction.

Figure 1 illustrates the propagation of the atomic wave packet through an optical potential as described by Eq. (5). Both subplots have the same parameters of the atomic velocity and laser intensity. From Fig. 1(a), we can see that the initial Gaussian wave packet is focused as it propagates through the potential. In Fig. 1(b), all the parameters are identical to those of Fig. 1(a) except that the propagation distance along the z-axis is longer. The Gaussian wave packet converges and then spreads as it passes through the region of the potential. We find that at a certain distance along the z-axis, the atom wave packet will be focused to form a high peak of probability. Thus in the experiment we should choose a proper distance between the standing wave (SW) field and the deposit substrate.

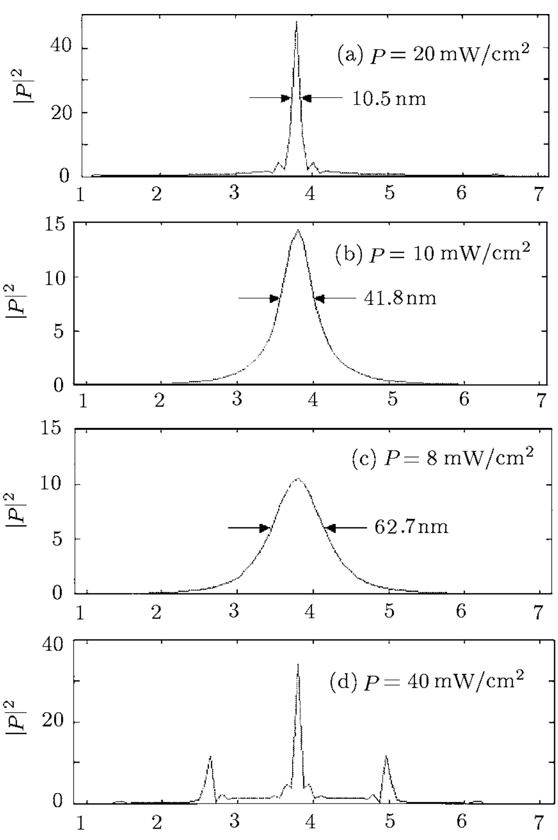

Fig. 3. Probability distribution of the atom wave packet at the same travel distance along the z-axis ($L = 78$, in units of laser beam radius) with the same atomic velocity ($v = 50\,\mathrm{m/s}$) in the region $-\lambda/4 \le x \le 3/4\lambda$ for various laser intensities.

Fig. 2 presents the distribution of the atomic possibility at the end of the z-axis (where the deposit substrate is placed). With the same parameters of the optical potential and the same propagation distance along the z-axis, three subplots are obtained. The atomic velocity is initialized with different values. It is very interesting to note a variety of the possibility peaks for different atomic velocities. Figure 2(a) with the atomic velocity of 50 m/s presents a sharp peak and a narrow full width at half maximum (FWHM) of 10.5 nm. In Fig. 2(b) with 70 m/s, the peak is lower and the FWHM is 31.7 nm. In Fig. 2(c) with 80 m/s, there is a much lower peak with a broader FWHM of 63.3 nm. We find that the velocity of the atom beam is critical in the atom focusing experiments. As Fig. 2 shows, the initial velocity spread in the atomic beam plays a significant role in determining the linewidth of atomic deposition. Thus we need to reduce the atomic velocity distribution to improve the effect of the atomic focusing in the atom-lithography experiment.

Figure 3 shows that when the velocity distribution is reduced at the point of 50 m/s, the intensity of the laser beam changes. In Fig. 3(a), we obtain a peak with a narrower FWHM of 10.5 nm when the laser intensity is $20\,\mathrm{mW/cm^2}$. When the laser intensity is reduced, as shown in Figs. 3(b) and 3(c), the FWHM of the peaks increases. In Fig. 3(d), where the light power is doubled, two additional small peaks appear, due to the fact that the atoms have been focused before they reach the substrate and then spread. Therefore, it is not useful to improve the quality of atom lithography by increasing the laser light power independently. In the experiment, the laser light power should be set at a proper fixed value.

In summary, we started from a two-dimensional Schrödinger equation and then reduced it to a one-dimensional equation to describe the behaviour of a Rb atomic beam in a focusing experiment. Considering the velocity distribution of the atoms and varying the power of the laser beam, we simulated the initial Gaussian atomic wave packet propagating through the laser light optical potential. This is helpful for us in understanding the properties of atomic focusing and will be useful in the future for the Rb atom-lithography experiment. Through our calculations, we have estimated the spot size of the Rb atom beam deposited onto the surface of the substrate. It has been found that two parameters, the atomic velocity and the intensity of the laser beam, played an important role in determining the deposition quality. In a future experiment, we should consider reducing the longitudinal velocity distribution. At the same time, we should also choose an appropriate laser power and deposition distance, so that a perfect peak can be formed through the deposition of the bulk of the atomic beam.

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