Lattice Confinement

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December 5, 2013

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1 Red-detuned lattice

A coherent gaussian beam propagating in the z direction and interfered with the retro-reflected beam creates a standing wave potential

$$U[\rho, z] = -U_0 e^{-\frac{2\rho^2}{W^2}} \cos^2[kz]$$
(1)

where U_0 is the lattice depth, which is positive for a red-detuned beam, $k = 2\pi/\lambda$ is the wave vector, W is the beam waist, $d = \lambda/2$ is the lattice spacing and $\rho^2 = x^2 + y^2$ is the radial variable.

1.1 Classical treatment

The minima of the lattice potential are located at $\mathbf{r}_{min} \equiv (\rho, z) = (0, \frac{n\pi}{2k})$, with *n* an integer. Using the formula $\omega = (M^{-1}\nabla^2 U|_{\mathbf{r}_{min}})^{1/2}$ for the trap frequency, with *M* the atomic mass, the axial and transverse (radial) confinements are

$$\omega_z = \sqrt{\frac{2U_0k^2}{M}} \quad \text{and} \quad \omega_\rho = \sqrt{\frac{4U_0}{W^2M}} \tag{2}$$

Sometimes it is convenient to express the lattice depth U_0 in units of the recoil energy $E_R \equiv \frac{\hbar^2 k^2}{2M}$.

$$\omega_z = \frac{2\sqrt{s}E_R}{\hbar} \quad \text{and} \quad \omega_\rho = \sqrt{\frac{4sE_R}{W^2M}} \tag{3}$$

1.2 Quantum correction

The lattice spacing in the z-direction is $\lambda/2$, which is comparable with the wavefunction spread at each lattice site. Therefore, we will treat the z-direction quantum mechanically and the ρ -direction classically.

The minima of the lattice potential are no longer $-U_0$ because of the zero point energy. Let us approximate each lattice site by a harmonic oscillator, which at the particular position z = 0 is

$$U[\rho, z] = -U_0 e^{-\frac{2\rho^2}{W^2}} + U_0 e^{-\frac{2\rho^2}{W^2}} k^2 z^2 + O(z^4)$$
(4)

$$= -U_0 e^{-\frac{2\rho^2}{W^2}} + \frac{1}{2} M(\omega_z[\rho])^2 z^2 + O(z^4)$$
(5)

where $\omega_z[\rho] \equiv \sqrt{\frac{2U_0k^2}{M}}e^{-\frac{\rho^2}{W^2}} \approx \sqrt{\frac{2U_0k^2}{M}} = \frac{2\sqrt{s}E_R}{\hbar}$ is the axial frequency at each lattice site. This frequency is associated with the bandgap of the periodic potential, and it coincides with eq. (2).

If we minimize the energy of the axial motion, the total energy of the system becomes

$$E[\rho] = -U_0 e^{-2\frac{\rho^2}{W^2}} + \frac{\hbar\omega_z[\rho]}{2}$$
(6)

$$= -U_0 e^{-2\frac{\rho^2}{W^2}} + \frac{\hbar}{2} \sqrt{\frac{2U_0 k^2}{M}} e^{-\frac{\rho^2}{W^2}}$$
(7)

The first term on the RHS is the classical energy. The second term is the zero-point energy from the quantum correction, which depends on the variable ρ . For $\rho \ll W$

$$E[\rho] = -U_0 \left(1 - 2\frac{\rho^2}{W^2}\right) + \frac{\hbar}{2} \sqrt{\frac{2U_0 k^2}{M}} \left(1 - \frac{\rho^2}{W^2}\right)$$
(8)

$$= -U_0 + \frac{\hbar}{2} \sqrt{\frac{2U_0}{M}} k + \left(2U_0 - \sqrt{\frac{U_0 \hbar^2 k^2}{2M}}\right) \frac{\rho^2}{W^2}$$
(9)

Hence, the transverse confinement is

$$\omega_{\rho} = \sqrt{\frac{4U_0}{W^2 M}} \left(1 - \sqrt{\frac{\hbar^2 k^2}{2MU_0}} \right)^{1/2} \tag{10}$$

$$=\sqrt{\frac{4sE_R}{W^2M}}\left(1-\frac{1}{2\sqrt{s}}\right)^{1/2}\tag{11}$$

1.3 3D lattice

If we extend the discussion above to three mutually orthogonal beams with identical waists and power, the lattice potential reads

$$U[x, y, z] = -U_0(e^{-2\frac{x^2 + y^2}{W^2}}\cos^2[kz] + e^{-2\frac{y^2 + z^2}{W^2}}\cos^2[kx] + e^{-2\frac{z^2 + x^2}{W^2}}\cos^2[ky])$$
(12)

From the eqs.(9,12), we deduce that the energy of the system after minimizing the quantum energy is

$$E[x, y, z] = const. + \frac{1}{2}M\omega_{\perp}^{2}(x^{2} + y^{2}) + \frac{1}{2}M\omega_{\perp}^{2}(y^{2} + z^{2}) + \frac{1}{2}M\omega_{\perp}^{2}(z^{2} + x^{2})$$
(13)

where the three axial frequencies are $\omega_{\perp} \equiv \sqrt{\frac{4sE_R}{W^2M}} \left(1 - \frac{1}{2\sqrt{s}}\right)^{1/2}$. The total confinement is then

$$\omega_{3D} = \sqrt{\frac{8sE_R}{W^2M}} \left(1 - \frac{1}{2\sqrt{s}}\right)^{1/2} \tag{14}$$

It is worth mentioning again that the frequency ω_{3D} arises because of the gaussian shape of the beams (ω_{3D} depends on the beam waist W). On the other hand, the confinement in each lattice site is

$$\omega_x = \omega_y = \omega_z \equiv \sqrt{\frac{2U_0k^2}{M}} \tag{15}$$

$$=\frac{2\sqrt{s}E_R}{\hbar}\tag{16}$$

2 Blue-detuned lattice

We can derive the equivalent results for a blue-detuned lattice. In this case, the lattice potential has the opposite sign of that in the eq.(1)

$$U[\rho, z] = U_0 e^{-\frac{2\rho^2}{W^2}} \sin^2[kz]$$
(17)

with $U_0 > 0$. The function $\cos^2[kz]$ was replaced by $\sin^2[kz]$ for the only purpose of making a Taylor expansion around z = 0 (both functions are equivalent except for a shift in the origin by half a lattice spacing)

$$U[\rho, z] = U_0 e^{-\frac{2\rho^2}{W^2}} k^2 z^2 + O(z^4)$$
(18)

$$= \frac{1}{2}M(\omega_z[\rho])^2 z^2 + O(z^4)$$
(19)

where $\omega_z[\rho] \equiv \sqrt{\frac{2U_0k^2}{M}}e^{-\frac{\rho^2}{W^2}}$. Next, we minimize the energy of the axial motion

$$E[\rho] = \frac{\hbar\omega_z[\rho]}{2} \tag{20}$$

$$=\frac{\hbar}{2}\sqrt{\frac{2U_0k^2}{M}}e^{-\frac{\rho^2}{W^2}}$$
(21)

$$=\frac{\hbar}{2}\sqrt{\frac{2U_0k^2}{M}} - \frac{\hbar}{2}\sqrt{\frac{2U_0k^2}{M}}\frac{\rho^2}{W^2}$$
(22)

The minus sign in the quadratic term implies that blue-detuned beams have a *de-confining* effect. The deconfinement is therefore

$$\omega_{\rho}^2 = -\frac{2E_R}{W^2 M}\sqrt{s} \tag{23}$$

and in a 3D cubic lattice

$$\omega_{3D}^2 = -\frac{4E_R}{W^2 M}\sqrt{s} \tag{24}$$