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# Trapping of cold atoms in optical lattices by the quadrupole force

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**Abstract**

Cold atoms are traditionally trapped by the dipole force in periodically spaced potential wells induced by the standing laser field. We derive here a theory beyond the conventional dipole approximation which provides field/atom coupling potential terms that so far have not been taken into consideration in theoretical or experimental studies. We show that for some atoms for specific laser parameters despite the absence of dipole transition *laser trapping is still possible due to the quadrupole force*. Illustrative numerical calculations for Ca and Na trapped by the quadrupole force are given.


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The possibility of trapping cold neutral atoms in periodic potentials formed by standing laser waves, so-called optical lattices, has opened a new subject of research. For reviews see for example Refs. [1–5] and references therein. Laser cooling and the formation of optical lattices were explained by the ability to influence the translational motion of neutral atoms by the laser induced dipole force [4]. Until now, the formation of optical lattices has been studied theoretically and experimentally exclusively due to the dipole interactions. An important question arises, however, on what happens when the dipole transition matrix element vanishes due to a symmetry property of the studied atomic system. This is the case, for example, when the laser frequency is detuned from an excited state which is associated with a $d$-type symmetry orbital whereas in the ground state the valence shell electron occupies an $s$-type symmetry orbital. Does this imply that in such a case atoms cannot be trapped because one cannot form an optical lattice? Or, must the only possible trapping mechanism be necessarily based just on a weak dipole coupling with other (far off-resonant) atomic levels?

The purpose of the present study is to demonstrate that it is possible to trap atoms exclusively due to the effect of quadrupole forces. We derive here the Hamiltonian of optical lattices without imposing the dipole approximation, and study the possibility of generating optical lattices due to the quadrupole contributions to the trapping potential which until now have been neglected. Two illustrative examples are presented explicitly. Namely, we show that by using realistic laser parameters the quadrupole force induced optical lattice can be formed and trap Ca and Na atoms.

Let us consider an atom interacting with a linearly polarized laser light. The light propagation direction is chosen to be $x$, and the field is assumed to oscillate along the $z$-direction. For the sake of simplicity and without loss of generality we describe the field free atomic Hamiltonian by an effective one electron model Hamiltonian, $\mathbf{H}_{\mathrm{el}}^{FF}$. The formulation given here can be extended in a straightforward manner to the general case of a many electron atom (or ion) interacting with an arbitrary (not necessarily linearly polarized) light pulse. Such a generalization will be elaborated elsewhere [6]. By switching from the laboratory frame coordinates to the relative $\vec{q} = (x, y, z)$ and center-of-mass (c.m.) $\vec{R} = (X, Y, Z)$ coordinates, one obtains the full Hamiltonian of an effective one electron atom in a linearly polarized laser field,

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$$\mathbf{H}(t) = -\frac{\hbar^2}{2M}\nabla_{\vec{R}}^2 + \mathbf{H}_{\rm el}^{FF}(\vec{q}) + \mathbf{V}_{\rm coup}(\vec{q},\vec{R},t) \tag{1}$$

with an interaction term $\mathbf{V}_{\rm coup}(\vec{q},\vec{R},t) = e(m_e c)^{-1}A_{m_e}\hat{p}_z + e^2(2m_e c^2)^{-1}A_{m_e}^{(2)} + e(cM)^{-1}A_M\hat{P}_Z + e^2(2(M-m_e)c^2)^{-1}A_M^{(2)}$. Here, the $A$-factors are defined in terms of the time, relative coordinate, and c.m. coordinate dependent vector potential $A(x,X,t)$, as follows: $A_{m_e} = [A(x\xi_1 + X,t) + (\xi_2/\xi_1)\times A(-x\xi_2 + X,t)]$; $A_M = [A(x\xi_1 + X,t) - A(-x\xi_2 + X,t)]$; $A_{m_e}^{(2)} = A^2(x\xi_1 + X,t)$ and $A_M^{(2)} = A^2(-x\xi_2 + X,t)$. The symbols $m_e$ and $M$ stand, respectively, for the mass of the electron and the atom, and parameters $\xi_1 = (M - m_e)/M$, $\xi_2 = m_e/M$. When the field intensity $I$ is weak ($I$ is proportional to the squared field amplitude) the linear interaction terms $A_{m_e}(x,X,t)\hat{p}_z$ and $A_M(x,X,t)\hat{P}_Z$ become dominant over the quadratic interaction terms $A_{m_e}^{(2)}$ and $A_M^{(2)}$ so that the latter two contributions can be neglected. Moreover, since $M \gg m_e$ it is clear that $\xi_1 \approx 1$ and thus the dominant term in $\mathbf{V}_{\rm coup}(\vec{q},\vec{R},t)$ is the first one. In summary, we conclude that the coupling between the c.m. and relative coordinates can be considered as

$$\mathbf{V}_{\rm coup}(\vec{q},\vec{R},t) = e(m_e c)^{-1}A_{m_e}(x,X,t)\hat{p}_z. \tag{2}$$

In standard treatments of the atom-field Hamiltonian the dependence of the vector potential on the relative coordinate has been neglected [7]. That is, $A(x+X,t) \sim A(X,t)$. Here, we do *not* use this so-called dipole approximation. Instead, the spatial dependence of the vector potential is taken into account, via the Taylor expansion around $x = 0$. An important question arises on what should be taken as the small parameter in such a Taylor series expansion. In the case when the laser intensity is low, the associated time dependent electronic wavefunctions are only slightly different from their field-free counterparts. Therefore, they possess exponentially small values for $q > a_0$, where $a_0$ stands for the size of the atom. For weak fields, as in our case, $a_0$ is essentially equal to the radius of the field free atom, $r_0$. Of course, in the presence of very strong fields $a_0$ varies with the intensity as the electron oscillates with the field. Roughly speaking we may think that the relevant radius of the atom is then $r_0 + \alpha_0$ where $\alpha_0 = (eA_0)^2/(c^2 m_e \omega_L)$ and $A_0$ is the field amplitude [8]. In order to find a qualitative criterion for convergence of our Taylor series expansion of $A(x+X,t)$, the above estimated atomic radius $a_0$ should be compared with the wavelength $\lambda$ of the laser. Clearly, $\lambda$ should get sufficiently large values such that $\lambda \gg a_0$. The small parameter of the considered Taylor series expansion is thus found to be $k_L a_0$, where $k_L = 2\pi/\lambda$.

Following the above discussion, when the wavelengths which constitute the dominant part of the laser pulse are sufficiently large, $\lambda \gg a_0$, the two leading order terms in the Taylor series expansion of the vector potential are given by

$$A(x+X,t) \sim A(X,t) + x\,\partial A(X,t)/\partial X. \tag{3}$$

The first term in Eq. (3) is the dipole term, whereas the second one is the quadrupole term which is taken here into consideration for the first time in contrast to other theoretical studies published up to now. Substituting Eq. (3) into formula (2) one finds that

$$\mathbf{V}_{\rm coup}(\vec{q},\vec{R},t) = \mathbf{V}_{\rm dip}(z,X,t) + \mathbf{V}_{\rm qd}(z,x,X,t), \tag{4}$$

where the dipole and quadrupole potential terms that couple the internal (electronic) and c.m. degrees of freedom are respectively given by, $\mathbf{V}_{\rm dip}(z,X,t) = (e/c)m_e^{-1}A(X,t)\hat{p}_z$ and $\mathbf{V}_{\rm qd}(z,x,X,t) = (e/c)m_e^{-1}[\partial A(X,t)/\partial X]x\hat{p}_z$.

Since the field oscillates periodically in time the Hamiltonian is time periodic with the period $T = 2\pi/\omega_L$ where $\omega_L$ is the laser frequency. In such a case the solutions of the time dependent Schrödinger equation are the Floquet solutions, similarly as the Bloch states are the solutions of the Schrödinger equation for spatially periodic potentials. Within the framework of the Floquet theory, the time averaged optical potential, $\bar{V}_{\rm opt}(X)$, is associated with the quasi-energy eigenvalue of the Floquet operator, $\mathcal{H}_F = -i\hbar\partial/\partial t + \mathbf{H}_{\rm el}^{FF}(\vec{q}) + \mathbf{V}_{\rm coup}(\vec{q},\vec{R},t)$, (for Floquet formalism see for example Ref. [9]),

$$\mathcal{H}_F \Phi_{\rm opt}^{\rm QE}(\vec{q},X,t) = \bar{V}_{\rm opt}(X)\Phi_{\rm opt}^{\rm QE}(\vec{q},X,t). \tag{5}$$

The eigenvalue solution of Eq. (5) provides the definition of the optical lattice potential. Strictly speaking, optical potentials for the atoms exist only in the adiabatic approximation where one can separate the atomic center of mass motion from the electronic motion (similarly to the Born–Oppenheimer or adiabatic approximation which separates the nuclear and electronic motions in molecules). Within the adiabatic approximation, our claim that the optical potential equals to an eigenenergy of the Floquet operator is *exact*. Of course, there are infinitely many eigenenergies and hence optical potentials (similarly to molecules where in each electronic state there is a potential for the vibrations). In Eq. (5) we have chosen that eigenenergy which correlates to the field-free atomic ground state. In the weak field limit we will show below that in the dipole case the same expression as that used in the literature results, whereas in the quadrupole case a novel expression for the quadrupole force induced optical lattice potential is obtained. Note however that for sufficiently strong fields, the literature expression (which is found to be a second order perturbation theory result) fails whereas the eigenenergy of the Floquet operator still provides an exact optical potential.

Let us derive now an analytical expression for the optical lattice potential which includes the leading order term beyond the dipole approximation. From Eq. (3) it is clear that the only information we need in order to go beyond the dipole approximation is $A(X,t)$ and its first order derivative with respect to the c.m. coordinate $X$. For atoms in a standing laser beam we have $A(X,t) = A_0(X)\cos(k_L X)\cos(\omega_L t)$, where $A_0(X)$ is the laser amplitude (which is allowed here to depend slowly upon $X$ due to finite spatial extension of a collimated laser beam in a realistic experiment), $\omega_L$ is the corresponding laser frequency, and $k_L = \omega_L/c$. Suppose that the atomic ground state $|g\rangle$ (with energy $\mathcal{E}_g^0$) is significantly coupled by the laser light only to a single excited electronic state $|e\rangle$ (with energy $\mathcal{E}_e^0 = \mathcal{E}_g^0 + \hbar\omega_{\rm atom}$). By following the "traditional" approach based upon the adiabatic elimination scheme [7], we obtain the time dependent optical lattice potential (including