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## Two-dimensional motion of cold atoms in a near-resonant annular laser beam: artificial two-dimensional molecules

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### Abstract

We develop the theory of the two-dimensional motion of cold atoms in a near-resonant annular laser beam. For a red-detuned field the laser beam provides an annular light shift potential and the atomic motion divides into vibrational and rotational normal motions analogous to a two-dimensional molecule. In the ground vibrational state we obtain an atom optics realization of a two-dimensional rotator. We illustrate the novel physics which may be explored with this system by showing that gravity acts analogously to a static electric field applied to a charged rotator.

### 1. Introduction

The planar rotator is a useful paradigm for the novel physics that can arise in quasi-two-dimensional (2D) physical systems, in which one dimension is frozen out using quantum confinement. The planar or 2D rotator consists of a particle which is constrained to move in a circular orbit around a fixed center. Silverman [1] has given a comprehensive discussion of the novel physics associated with the quantum 2D rotator including the symmetry breaking properties in external electromagnetic fields, mesoscopic conductivity of 2D rings in vector potentials [2], and the relevance of the 2D rotator to the issue of composite quasi-particles with fractional statistics [3,4]. Current experimental realizations of a 2D rotator include a p-electron in benzene [5], whose spectrum can be interpreted in terms of transitions between rotator eigenstates, and mesoscopic 2D rings of conducting material [6].

In this paper we discuss a possible atom optics realization of a 2D rotator involving a laser cooled two-level atom tightly bound by the light shift (optical) potential [7] supplied by a near-resonant, annular laser beam. This configuration is closely related to previously demonstrated optical traps for laser cooled atoms formed by the light shift potential in a tightly focused Gaussian beam [8]. Here, however, the light field supplies an annular as opposed to a Gaussian light shift potential. Studies of atomic motion in periodic arrays of light shift potential wells formed by laser standing waves, so-called optical lattices, have recently revealed a close similarity to the motion of electrons in a solid, and now show promise as model systems in which to study condensed matter phenomena [9]. Similarly, the wavelength sized annular trap proposed here approximates a two-dimensional molecular system, with a spectrum of rotational-vibrational eigenstates. We expect this “artificial 2D molecule” to provide a new, well controlled model system for molecular physics, with the obvious advantage that the con-

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fining potential and spectrum of eigenstates is exactly calculable. In its ground vibrational state the system yields a realization of the 2D rotator. To illustrate the novel physics which can be explored using this system we show that the external force of gravity acts analogously to the Stark effect for a charged rotator with an applied electric field [1].

The remainder of this paper is organized as follows: Our basic model describing 2D atomic motion is given in Section 2 along with a discussion of the energy eigenstates of the system. Section 3 introduces the idea of artificial 2D molecules, and the ideal limit of a rotator incorporating the effects of gravity are discussed in Section 4. Finally, our Summary and Conclusions are given in Section 5.

## 2. Theoretical model

In this section we describe our theoretical model. First we give the Hamiltonian for our system, and then discuss the angular momentum of the system and the energy eigenstates.

### 2.1. Basic equations

The basic model consists of a sample of cold atoms which are constrained to move in two dimensions  $\mathbf{R}_\perp = (X, Y) = (R, \theta)$  perpendicular to a travelling-wave laser beam of frequency  $\omega_L$  propagating along the  $Z$ -axis. This could be achieved, for example, by using a one-dimensional off-resonant optical lattice also along the  $Z$ -axis [9]. For an optical lattice formed by a red-detuned field the atoms will be confined longitudinally in the light shift potentials around the anti-nodes of the standing-wave laser. We assume that any new energy scales introduced into the system by the travelling-wave laser are small compared to the longitudinal vibrational energy, so that the atoms occupy the ground vibrational state of their respective longitudinal potential wells, thus producing quasi-two-dimensional atomic motion at the anti-nodes of the optical lattice.

The transverse profile of the travelling-wave laser field is the  $\text{TEM}_{01}^*$  Laguerre-Gaussian mode with azimuthal variation  $e^{i\ell\theta}$ , or doughnut mode [10,11], which has a phase singularity at its center with topological charge  $\ell = \pm 1$ , and the field is assumed right

circularly polarized. Then in cylindrical coordinates we write the electric field operator as [12]

$$\begin{aligned} \hat{\mathbf{E}}(\mathbf{R}, t) &= i\sqrt{\frac{\hbar\omega_L}{2\epsilon_0 L}} \left[ \mathbf{e}_+ \hat{a} f(R, Z) \right. \\ &\quad \times e^{i(k_L Z + \ell\theta + \Theta(Z) - \omega_L t)} - \text{h.c.} \left. \right] \\ &= \frac{1}{2} \mathbf{e}_+ \hat{\mathbf{E}}^+(\mathbf{R}_\perp, Z) e^{-i\omega_L t} + \text{h.c.}, \end{aligned} \quad (1)$$

where  $\mathbf{e}_+$  is the right circular polarization unit vector,  $\hat{a}$  and  $\hat{a}^\dagger$  are the field creation and annihilation operators,  $[\hat{a}, \hat{a}^\dagger] = 1$ , a caret being used throughout to denote an operator,  $k_L = \omega_L/c$ ,  $L$  is the quantization length along  $Z$ , and  $\Theta(Z)$  is the Guoy phase-shift [10]. Here  $f(R, Z)$  is the normalized transverse field profile including the amplitude distribution and phase curvature

$$f(R, Z) = \frac{2R}{\sqrt{\pi}w(Z)} e^{(ik_L R^2/2r(Z) - R^2/w^2(Z))}, \quad (2)$$

where  $r(Z)$  is the radius of curvature and  $w(Z)$  the spot size. Also  $1/r(0) = 0$  and  $w(0) = w_0$ , so that  $f(R, 0)$  is real at the beam focus [10,11].

In recent work it has been shown that in addition to the spin angular momentum of the photon, which is equal to  $\pm\hbar$ , it is also useful to endow the photon with an external orbital angular momentum associated with its electric field envelope [13–18]. Although not strictly applicable in quantum electrodynamics [12], this notion of separating the photon angular momentum into spin and orbital components is appropriate in the paraxial approximation which applies when the focused beam waist is large compared to an optical wavelength [14,16,19],  $k_L w_0 \gg 1$ , a condition we assume is met here. For the field in Eq. (1) the orbital angular momentum is  $\hbar\ell$  [13,14,16].

The laser field is dipole coupled to the system of atoms. For concreteness we consider the  $J = 2 \rightarrow J = 3$  hyperfine levels of  $^{23}\text{Na}$  ( $3S_{1/2} \rightarrow 3P_{3/2}$  at 589.59 nm). Then if the Na atoms are initially prepared by optical pumping with resonant right-polarized light, we may treat the atoms as two-level systems with excited and ground states

$$|e\rangle = |J = 3, m = 3\rangle, \quad |g\rangle = |J = 2, m = 2\rangle, \quad (3)$$

and energy difference  $E_e - E_g = \hbar\omega_{eg}$ . Spontaneous emission is neglected throughout under the condition of off-resonant excitation so that only stimulated transitions between the levels are considered. Then the two

levels are coupled only by the incident right-circular polarized light, and the dipole selection rules  $\delta J = \pm 1$ , and  $\delta m = 0, \pm 1$  are obeyed for stimulated absorption (+1) and emission (−1) of right-circular polarized photons.

To describe the dipole interaction between the atoms and the travelling-wave laser field we must consider that the atoms are confined to two-dimensional planes at many longitudinal positions if an optical lattice is employed. However, the dipole interaction will be strongest within a Rayleigh range  $Z_R = k_L w_0^2$  of the laser beam focus at  $Z = 0$ . (We assume that the spot size and Rayleigh range of the standing-wave laser are much larger than those of the travelling-wave). Thus to investigate the two-dimensional motion of the cold atoms we shall consider the plane  $Z = 0$  as representative of the behavior around the laser focus. The evolution of the atom-field system is then governed by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi_s(t)\rangle = \hat{H}_s |\psi_s(t)\rangle, \tag{4}$$

and in the rotating-wave and dipole approximations the Hamiltonian is [7,20]

$$\hat{H}_s = \hbar \hat{a}^\dagger \hat{a} + \hat{P}_\perp^2 / 2M + \hbar \omega_{eg} |e\rangle\langle e| - \frac{1}{2} [d \hat{E}^+(\hat{\mathbf{R}}_\perp, 0) |e\rangle\langle g| + \text{h.c.}]. \tag{5}$$

Here  $\hat{P}_\perp$  is the transverse momentum operator for the center-of-mass motion of the atom,  $\hat{\mathbf{R}}_\perp$  the center-of-mass position operator,  $M$  is the atomic mass, and  $d = \langle e | \mathbf{d} \cdot \mathbf{e}_+ | g \rangle$  is the dipole matrix element which we take as real without loss of generality. In writing Eq. (5) we have assumed that the  $Z$ -axis is vertical so that gravitational effects are uniform over the two-dimensional transverse plane. In addition, the Hamiltonian (5) includes only stimulated transitions involving the single electromagnetic mode with field profile (2). Thus the theory is only valid in the limit of large detunings where spontaneous emission can be neglected.

By observing that the excitation number operator  $\hat{N} = \hat{a}^\dagger \hat{a} + |e\rangle\langle e|$  is a constant of motion, we introduce an interaction picture defined by the unitary transformation

$$|\psi_s(t)\rangle = e^{-i\hat{N}\omega_L t} |\psi(t)\rangle. \tag{6}$$

In this interaction picture the Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle, \tag{7}$$

with the Hamiltonian

$$\hat{H} = \hat{P}_\perp^2 / 2M - \hbar \Delta |e\rangle\langle e| - \frac{1}{2} [d \hat{E}^+(\hat{\mathbf{R}}_\perp, 0) |e\rangle\langle g| + \text{h.c.}], \tag{8}$$

where the laser-atom detuning is  $\Delta = \omega_L - \omega_{eg}$ . To proceed we write the state vector as a sum over disconnected manifolds

$$|\psi(t)\rangle = \sum_n |\psi_n(t)\rangle, \tag{9}$$

where in the coordinate representation

$$\langle \mathbf{R}_\perp | \psi_n(t) \rangle = \psi_{e,n}(\mathbf{R}_\perp, t) |e, n-1\rangle + \psi_{g,n}(\mathbf{R}_\perp, t) |g, n\rangle. \tag{10}$$

Here the state  $|g, n\rangle$  describes the atom in its ground electronic state and the field in a number state with  $n$  photons, and  $|e, n-1\rangle$  describes the atom in its excited electronic state and the field in a number state with  $(n-1)$  photons. In the dipole approximation the manifolds  $|\psi_n(t)\rangle$  for different values of  $n$  do not couple in the absence of spontaneous emission [7,21]. Then substituting the wave function (10) into the Schrödinger equation (7) and projecting onto the states  $|e, n-1\rangle$  and  $|g, n\rangle$  we obtain the following coupled equations

$$i\hbar \frac{\partial \psi_{e,n}}{\partial t} = -\frac{\hbar^2}{2M} \nabla_\perp^2 \psi_{e,n} - \hbar \Delta \psi_{e,n} - \frac{i}{2} d \mathcal{E}_n(R) e^{i\ell\theta} \psi_{g,n},$$

$$i\hbar \frac{\partial \psi_{g,n}}{\partial t} = -\frac{\hbar^2}{2M} \nabla_\perp^2 \psi_{g,n} + \frac{i}{2} d \mathcal{E}_n(R) e^{-i\ell\theta} \psi_{e,n}, \tag{11}$$

where

$$\nabla_\perp^2 = \frac{\partial^2}{\partial R^2} + \frac{1}{R} \frac{\partial}{\partial R} + \frac{1}{R^2} \frac{\partial^2}{\partial \theta^2}, \tag{12}$$

is the transverse Laplacian, and we have defined

$$\mathcal{E}_n(R) = \sqrt{\frac{8\hbar\omega_L n}{\epsilon_0 \pi L w_0^2}} \left(\frac{R}{w_0}\right) e^{-R^2/w_0^2}$$

$$= \sqrt{2} e^{1/2} \mathcal{E}_{0,n} \left(\frac{R}{w_0}\right) e^{-R^2/w_0^2}, \tag{13}$$

where  $\mathcal{E}_{0,n}$  is the electric field at the peak of the annular beam  $R = w_0/\sqrt{2}$ .

### 2.2. Angular momentum of the system

Here we obtain the external angular momentum operator associated with the orbital angular momentum of the photons and the center-of-mass motion of the atom, conservation of the angular momentum associated with the photon spin and the internal electronic states of the atom being ensured by the dipole selection rules [22]. For the present case of two-dimensional motion in the  $(R, \theta)$  plane the angular momentum is directed along the  $Z$ -axis. The external angular momentum operator along the  $Z$ -axis is then

$$\hat{J}_{\text{ext}} = \hat{L} + \hbar \ell \hat{a}^\dagger \hat{a}, \quad (14)$$

where  $\hat{L} = -i\hbar \partial / \partial \theta$  is the orbital angular momentum operator for the atoms, and we have used the fact that the light field carries an orbital angular momentum  $\hbar \ell$  per photon,  $\hat{a}^\dagger \hat{a}$  being the photon number operator. Physically,  $\hat{J}_{\text{ext}}$  is the generator of rotations around the  $Z$ -axis for the external degrees of freedom of the combined atom-field system.

It is straightforward to verify that  $\hat{J}_{\text{ext}}$  commutes with the Hamiltonian and is therefore a constant of motion. In addition, the excitation number operator  $\hat{N}$  commutes with both the Hamiltonian and  $\hat{J}_{\text{ext}}$ . Thus we have three operators at our disposal which can be used as members of a complete set of commuting observables [23].

### 2.3. Energy eigenstates

Eqs. (11) have energy eigenstates of the form

$$\begin{pmatrix} \psi_{e,n}(R, \theta, t) \\ \psi_{g,n}(R, \theta, t) \end{pmatrix} = e^{-iE_{npq}t/\hbar} \begin{pmatrix} u_{npq}(R) e^{i(p+\ell)\theta} \\ i v_{npq}(R) e^{ip\theta} \end{pmatrix}, \quad (15)$$

which yields the following coupled equations for the eigensolutions

$$\begin{aligned} E_{npq} u_{npq} &= -\frac{\hbar^2}{2M} \left( \frac{d^2}{dR^2} + \frac{1}{R} \frac{d}{dR} - \frac{(p+\ell)^2}{R^2} \right) u_{npq} \\ &\quad - \hbar \Delta u_{npq} - \frac{d\mathcal{E}_n(R)}{2} v_{npq}, \end{aligned} \quad (16)$$

$$\begin{aligned} E_{npq} v_{npq} &= -\frac{\hbar^2}{2M} \left( \frac{d^2}{dR^2} + \frac{1}{R} \frac{d}{dR} - \frac{p^2}{R^2} \right) v_{npq} \\ &\quad - \frac{d\mathcal{E}_n(R)}{2} u_{npq}. \end{aligned} \quad (17)$$

Here  $p$  is constrained to be an integer so that the wave function is single-valued, and the label  $q = \{q_1, q_2, \dots\}$  accounts for the remaining quantum numbers required to specify the eigenstates uniquely. The eigensolution (15) is a superposition of the atomic ground electronic state with center-of-mass angular momentum  $\hbar p$  and the excited state with angular momentum  $\hbar(p + \ell)$ . This superposition is dictated by the fact that the center-of-mass angular momentum of the atom changes by  $\hbar \ell$  upon absorbing a photon.

The energy eigenstates (15) are also eigenstates of the excitation number operator and external angular momentum operator with expectation values

$$\langle \psi_n(t) | \hat{N} | \psi_n(t) \rangle = \langle \hat{N} \rangle = n, \quad (18)$$

and

$$\langle \psi_n(t) | \hat{J}_{\text{ext}} | \psi_n(t) \rangle = \hbar(\ell n + p). \quad (19)$$

As expected of the generator of rotations, the eigenvalues of the external angular momentum in Eq. (19) are strictly integer multiples of  $\hbar$ . In contrast, the expectation value of the orbital angular momentum operator for the atoms is  $\langle \hat{L} \rangle = \hbar(p + \ell P_{e,npq})$ ,  $P_{e,npq} = \int 2\pi R dR |u_{npq}(R)|^2$  being the excited state population, which need not be an integer multiple of  $\hbar$  when the excited state population is non-zero. This observation is central to the recent proposal [24] that composite particles consisting of an atom trapped on an electromagnetic vortex (or more generally a field with orbital angular momentum) have fractional orbital angular momentum and should obey fractional statistics, i.e. they are anyons [3,4]. However, in this paper we consider the limit of large atom-field detunings (see Section 3) so that the excited state population is negligible, in which case the orbital angular momentum assumes values which are integer values of  $\hbar$ . A consistent treatment of the fractional orbital angular momentum would entail introducing spontaneous emission concomitantly with the excited state population, and this is beyond the scope of the present paper.

The quantum numbers  $n$ ,  $p$ , and  $q$  are used to label the energy eigenstates in Eq. (15). Clearly,  $n$  and  $p$  are the eigenvalues associated with the operators  $\hat{N}$  and  $(\hat{J}_{\text{ext}} - \hbar \ell \hat{N}) / \hbar$ . If for fixed  $n$  and  $p$  the eigenenergies of Eqs. (16) and (17) are non-degenerate, then each eigenstate can be labeled by a single integer  $q$ . In this case the Hamiltonian, external angular momen-

tum, and excitation number operator form a complete set of commuting operators so that a set of three quantum numbers is expected for each eigenstate [23].

### 3. Artificial two-dimensional molecules

In this section we analyze the energy eigenstates of the two-dimensional atomic motion for large detunings using a harmonic oscillator approximation to the radial motion near the minimum of the annular potential. The atomic motion then naturally divides into vibrational and rotational normal motions, completely analogous to that of a two-dimensional molecule.

#### 3.1. Large detuning approximation

Here we consider the limit of large detunings for which  $|\Delta|$  is assumed much greater than the peak Rabi frequency  $\mathcal{R}_{0,n} = d\mathcal{E}_{0,n}/\hbar$  and the atomic recoil frequency  $\omega_R = \hbar k_L^2/2M$ . In this case, and assuming that the atoms are predominantly in their ground electronic state, the excited state population may be neglected, and the pair of Eqs. (11) reduces to the scalar equation

$$i\hbar \frac{\partial \psi_{g,n}}{\partial t} = -\frac{\hbar^2}{2M} \nabla_{\perp}^2 \psi_{g,n} + \frac{d^2 \mathcal{E}_n^2(R)}{4\hbar \Delta} \psi_{g,n}. \quad (20)$$

Here we are exclusively interested in the case that the atoms are in their ground state since spontaneous emission will render unobservable the eigenstates which are predominantly in their excited state. Then substituting the eigensolution (15) in Eq. (20) we obtain the following scalar eigenequation

$$E_{npq} v_{npq} = -\frac{\hbar^2}{2M} \left( \frac{d^2}{dR^2} + \frac{1}{R} \frac{d}{dR} - \frac{p^2}{R^2} \right) v_{npq} + U_n(R) v_{npq}, \quad (21)$$

with the light shift potential [7]

$$U_n(R) = \frac{d^2 \mathcal{E}_{0,n}^2}{2\hbar \Delta} \left( \frac{R}{w_0} \right)^2 e^{(1-2R^2/w_0^2)}. \quad (22)$$

The eigenenergies of this scalar equation are non-degenerate for fixed  $n$  and  $p$ , in which case the eigensolutions may be labeled using  $q = 0, 1, 2, \dots$ . In this limit the quantum number  $q$  is the number of radial nodes in the ground state wave function, and it plays the role of a radial vibrational quantum number. From

Eq. (21) it is likewise clear that  $p$  is the rotational quantum number for the atom. Finally,  $n$  is the number of photons in the field. For a coherent state field with a large photon number, so that photon number fluctuations are negligible, we may safely replace  $n$  by the mean photon number  $\bar{n}$ . Thus in the following discussion we shall drop the explicit  $n$  subscript, and replace  $\mathcal{E}_{0,n}$  by  $\mathcal{E}_0$ , the classical field amplitude.

Here we consider the case of a red-detuned laser field,  $\Delta < 0$ , and the annular laser beam then produces an annular light-induced potential of the form shown by the solid line in Fig. 1. The potential minimum occurs at a radius  $R_{\min} = w_0/\sqrt{2}$ .

#### 3.2. Harmonic oscillator approximation

We now approximate the light-induced potential in Fig. 1 by a harmonic oscillator around the potential minimum

$$U(R) \approx U_{\min} + \frac{1}{2} M \Omega^2 (R - R_{\min})^2, \quad (23)$$

where  $U_{\min} = d^2 \mathcal{E}_0^2 / 4\hbar \Delta$  is the potential minimum, the oscillation frequency is  $\Omega^2 = 2d^2 \mathcal{E}_0^2 / M\hbar |\Delta| w_0^2$ , and the corresponding harmonic oscillator ground state width is  $\Delta R = \sqrt{\hbar/M\Omega}$ . The harmonic oscillator approximation is valid if  $\Delta R \ll R_{\min}$  so that the atomic wave function is well localized around the potential minimum. Then the term  $d^2 v/dR^2$  will be of order  $v_0/\Delta R^2$ , with  $v_0$  the characteristic value of the wave function around the potential minimum,  $R^{-1} dv/dR$  will be of order  $v_0/R_{\min} \Delta R$ , and  $p^2 v/R^2$  will be order

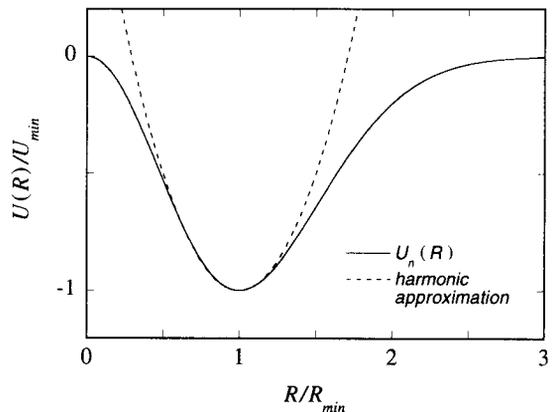


Fig. 1. Light shift potential  $U(R)$  for a red-detuned laser field showing the potential minimum at  $R = w_0/\sqrt{2}$ . The dotted line shows the harmonic oscillator approximation to the full potential.

$p^2 v_0 / R_{\min}^2$ . Thus, the kinetic energy term in Eq. (21) is dominated by the second-order derivative and the other two terms may be treated as perturbations. The leading order approximation to Eq. (21) is then

$$E_{pq}^{(0)} v_{pq}^{(0)} = -\frac{\hbar^2}{2M} \frac{d^2}{d\xi^2} v_{pq}^{(0)} + \frac{1}{2} M \Omega^2 \xi^2 v_{pq}^{(0)} + U_{\min} v_{pq}^{(0)}, \quad (24)$$

where  $\xi = R - R_{\min}$ , and in view of the above approximations we may extend this variable over the full range  $\{-\infty, \infty\}$  without significant error. Since the dynamics in the  $\xi$  variable is reduced to a one-dimensional harmonic oscillator the eigensolutions are given by

$$v_{pq}^{(0)}(\xi) = \left( \frac{1}{\pi \Delta R^2} \right)^{1/4} \frac{1}{\sqrt{2^q q!}} e^{-\xi^2/2\Delta R^2} H_q(\xi/\Delta R), \quad (25)$$

where  $H_q(y)$  are Hermite polynomials, and the eigenenergies are given by  $E_{pq}^{(0)} = U_{\min} + \hbar\Omega(q+1/2)$ . If we now reintroduce the kinetic energy terms previously discarded from Eq. (21) as first-order perturbations, then we obtain the eigenenergies correct to first-order as

$$E_{pq} = U_{\min} + \hbar\Omega \left( q + \frac{1}{2} \right) + \frac{\hbar^2 p^2}{2MR_{\min}^2}. \quad (26)$$

The motion therefore decouples into two normal modes: Vibrational motion in the radial  $\xi$  variable with quantum number  $q$ , and rotational motion with quantum number  $p$ . These energies are precisely those of a *two-dimensional molecule*. That is, if we consider a diatomic molecule whose motion is confined to be two-dimensional then in the Born-Oppenheimer approximation we would expect rotational-vibrational energy levels given precisely by Eq. (26).

The theory developed here assumes that the excited electronic state is negligibly populated. Under the approximations used here the excited state population along the top of the annular beam is given by  $(d\mathcal{E}_0/2\hbar\Delta)^2$ , and this should be much less than unity. This quantity also dictates the magnitude of the errors incurred by ignoring the excited state population. In particular, we must ensure that the rotational energies in Eq. (26), obtained in first-order perturbation theory, are not below these errors. For Eq. (26) to be consistent we require

$$1 \gg \frac{(\hbar^2 p^2 / 2MR_{\min}^2)}{\hbar\Omega} \gg \left( \frac{d\mathcal{E}_0}{2\hbar\Delta} \right)^2, \quad (27)$$

otherwise the excited state population must be included explicitly to deal with the rotational levels. Even if this is satisfied, in order for the lower energy rotational states to be spectroscopically resolvable the transition frequencies must be greater than the photon scattering rate,  $\gamma_s = (\Gamma/2)(d\mathcal{E}_0/2\hbar\Delta)^2$ , where  $\Gamma$  is the inverse spontaneous lifetime of the excited state. Thus for a transition with  $\Delta p = 1$ , we require  $E_{p+1,q} - E_{p,q} = (2p+1)\hbar^2/2MR_{\min}^2 > \hbar\gamma_s$ . Furthermore, if we want the  $p \rightarrow p+1$  transition to be resolvable from the  $p+1 \rightarrow p+2$  transition and so on, we have the more stringent condition

$$\frac{\hbar^2}{MR_{\min}^2} > \hbar\gamma_s = \frac{\hbar\Gamma}{2} \left( \frac{d\mathcal{E}_0}{2\hbar\Delta} \right)^2. \quad (28)$$

This is basically a condition on the magnitude of the detuning required so that transitions between rotational states can be resolved individually and from each other.

### 3.3. Numerical results and discussion

We have obtained numerical solutions for energy eigenstates using both the pair of Eqs. (16) and (17), and also the approximate scalar Eq. (21). For the numerical results presented here for large red-detunings the pair of equations and the scalar equation yield the same energy eigenvalues to very high accuracy. Here we concentrate on the scalar equation.

To facilitate numerical simulations the radial coordinate is scaled to the input spot size  $\eta = R/w_0$ , and the energies are scaled to  $E_0 = \hbar^2/2Mw_0^2 = (k_L w_0)^{-2} E_R$ , with  $E_R = \hbar^2 k_L^2/2M$  the recoil energy. Then Eq. (21) becomes

$$\epsilon_{pq} v_{pq} = - \left( \frac{d^2}{d\eta^2} + \frac{1}{\eta} \frac{d}{d\eta} - \frac{p^2}{\eta^2} \right) v_{pq} + K \eta^2 e^{-2\eta^2} v_{pq}, \quad (29)$$

where  $\epsilon_{pq} = E_{pq}/E_0$ , and

$$K = \frac{2e}{E_0} \frac{d^2 \mathcal{E}_0^2}{4\hbar\Delta} = 2e (k_L w_0)^2 \left( \frac{U_{\min}}{E_R} \right). \quad (30)$$

Thus, the solutions of the scalar equation are characterized by the single parameter  $K$ . For the results pre-

sented below we set  $w_0 = 10\lambda_L$ , and  $U_{\min} = -9.4E_R$ , giving  $K = -2 \times 10^5$ . For Na atoms this corresponds to a light shift potential well depth of  $U_{\min} = 22.4 \mu\text{K}$ . These values are representative of reasonable beam focusing while still being in the paraxial approximation, and a moderate light shift potential depth. If anything, this value of  $K$  may be considered small.

In the harmonic oscillator approximation the energy eigenvalues of Eq. (29) become

$$\epsilon_{pq} = \frac{U_{\min}}{E_0} + (q + \frac{1}{2})\sqrt{-8K/e} + 2p^2, \quad (31)$$

where we identify  $\hbar\Omega/E_0 = \sqrt{-8K/e}$ . In terms of the dimensionless spatial variable  $\eta$  we have  $\eta_{\min} = R_{\min}/w_0 = 2^{-1/2}$ , and  $\Delta\eta = \Delta R/w_0 = \sqrt{-e/4K}$ . Thus, the condition  $R_{\min} \gg \Delta R$  for the harmonic oscillator approximation to be valid becomes  $K \ll -1$ , and this is well obeyed for the example chosen here with  $K = -2 \times 10^5$ . This means that the harmonic oscillator approximation is applicable to those quantum states which are localized around the potential minimum, i.e. those with smaller values of  $p, q$ .

Fig. 2 shows the scaled vibrational energy difference  $\epsilon_{pq} - \epsilon_{p0}$  versus the vibrational quantum number  $q$  for  $p = 0$  (squares) and  $p = 20$  (crosses). From the harmonic oscillator approximation we expect  $\epsilon_{pq} - \epsilon_{p0} = q\sqrt{-8K/e}$ , independent of  $p$ , and this linear relation is well obeyed in Fig. 2. This is to be expected since the vibrational energy is the leading-

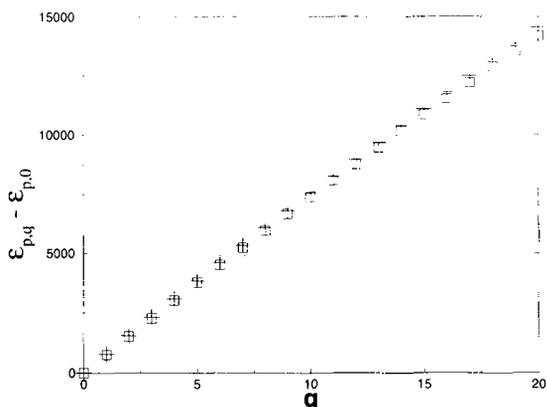


Fig. 2. Vibrational energies for  $K = -2 \times 10^5$ : Scaled vibrational energy difference  $\epsilon_{pq} - \epsilon_{p0}$  versus the vibrational quantum number  $q$  for  $p = 0$  (squares) and  $p = 20$  (crosses). The predicted slope is  $\sqrt{-8K/e} = 767$ , in excellent agreement with the numerics.

order contribution to the energy. The slope of the energy curve  $(\epsilon_{pq} - \epsilon_{p0})/q$  was found to be in excellent agreement with the theoretical prediction  $\sqrt{-8K/e} = 767$ .

Fig. 3a shows the scaled rotational energy difference  $\epsilon_{pq} - \epsilon_{0q}$  versus the rotational quantum number squared  $p^2$  for  $q = 0$  (squares) and  $q = 20$  (crosses). From the harmonic oscillator approximation we obtain  $\epsilon_{pq} - \epsilon_{0q} = 2p^2$ , independent of  $q$ . This relation is well obeyed for  $q = 1$ , but deviations are evident for  $q = 20$ . The source of the discrepancy is rotational-vibrational coupling and anharmonicity of the potential well which are beyond the harmonic oscillator approximation. Nonetheless, from Fig. 3a we

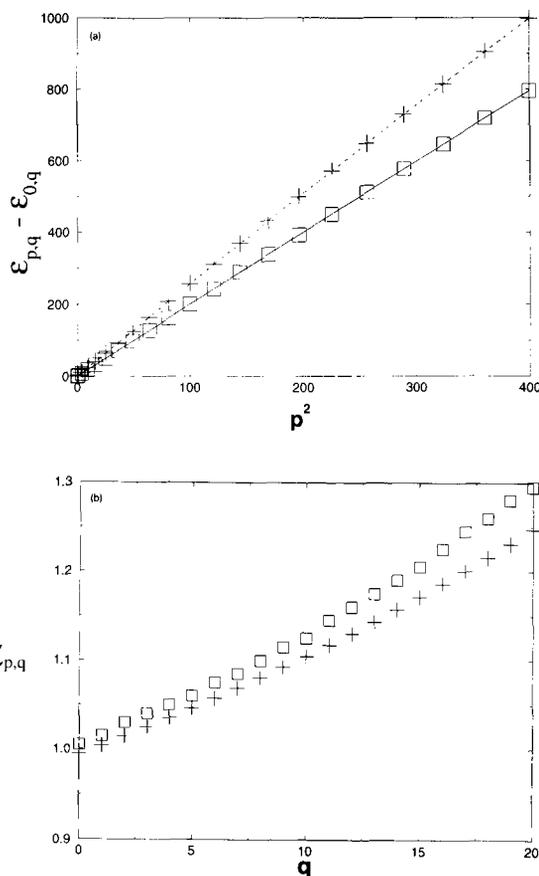


Fig. 3. Rotational energies for  $K = -2 \times 10^5$ : (a) Scaled rotational energy difference  $\epsilon_{pq} - \epsilon_{0q}$  versus the rotational quantum number squared  $p^2$  for  $q = 0$  (squares) and  $q = 20$  (crosses), and (b) slope of the energy curve  $\chi_{pq} = (\epsilon_{pq} - \epsilon_{0q})/2p^2$  versus  $q$  for  $p = 1$  (squares) and  $p = 20$  (crosses).

see that even for  $q = 20$  the relation between the rotational energy difference and  $p^2$  is still very close to linear, so that we consider an expression of the form  $\epsilon_{pq} - \epsilon_{0q} = 2\chi_{pq}p^2$ . Fig. 3b shows  $\chi_{pq}$  versus  $q$  for  $p = 1$  (squares) and  $p = 20$  (crosses). For  $q = 20$  we have  $\chi_{1,20} = 1.3$  and  $\chi_{20,20} = 1.25$ , whereas for  $p = 1$  we have  $\chi_{1,1} = 1.0$  and  $\chi_{1,20} = 1.3$ . This example illustrates the point that  $\chi_{pq} \approx \chi_q$  depends mainly on the vibrational quantum number  $q$ , which is to be expected since the leading-order solutions in the harmonic oscillator approximation are the vibrational modes (see Eq. (26)). Thus, for a given vibrational quantum number  $q$  the rotational series is still close to that of an ideal 2D rotator. In particular, we expect this approximation to hold until  $\hbar\Omega \leq \hbar^2 p^2 / 2MR_{\min}^2$ , at which point the perturbation expansion fails since the rotational energy is comparable with the vibrational energy (see Eq. (27)). In terms of dimensionless quantities this yields  $p \geq (-K)^{1/4}$  for the failure of the rotational series, or  $p \geq 20$  for  $K = -2 \times 10^5$ . Then in dimensional units the rotational-vibrational energy eigenvalues are to a good approximation

$$E_{pq} = U_{\min} + \hbar\Omega \left( q + \frac{1}{2} \right) + \chi_q \frac{\hbar^2 p^2}{2MR_{\min}^2}, \quad (32)$$

where  $\chi_q$  should be determined numerically in general.

We now resort to dimensional quantities to discuss the various scales for a potential experiment in Na, and we set  $\chi_q = 1$  for illustration. In particular we have for the vibrational frequency

$$\nu = \Omega / 2\pi = \frac{4}{k_L w_0} \sqrt{\frac{-U_{\min}}{E_R}} \nu_R, \quad (33)$$

for the rotational frequencies

$$\frac{E_{pq} - E_{0q}}{2\pi\hbar} = \frac{2p^2}{(k_L w_0)^2} \nu_R, \quad (34)$$

and for the harmonic oscillator ground state width

$$\Delta R = \frac{1}{\sqrt{k_L w_0}} \left( \frac{-U_{\min}}{E_R} \right)^{-1/4} R_{\min}, \quad (35)$$

with  $R_{\min}$  the radius of the potential minimum as before. For our nominal values of  $w_0 = 10\lambda_L$  and  $U_{\min}/E_R = -9.4$ , and using  $\nu_R = \omega_R / 2\pi = 25$  kHz for Na, we obtain  $\nu = 5$  kHz, the frequency splitting

between the  $p$  and  $p + 1$  rotational levels is  $\Delta\nu_p = 12(2p + 1)$  Hz, and  $\Delta R = 0.07R_{\min}$ . First we note that since  $\Delta R < R_{\min}$  the harmonic oscillator approximation is valid. Next, it is clear that the rotational frequency splitting is very small, on the order of a few tens of Hz, making spectroscopy difficult at best. However, by using a tighter focused beam, say  $w_0 = 2\lambda_L$ , then the frequency splitting becomes  $\Delta\nu_p = 305(2p + 1)$  Hz, which for  $p = 10$  now yields 6 kHz, which is perhaps realistic for observation. The rotational spectrum can in principle be measured by using Raman spectroscopy with two fields with their orbital angular momentum different by unity. A stimulated Raman transition involves absorption of a photon from one beam followed by stimulated emission into the other; if these photons differ only by their orbital angular momentum then the process will transfer an orbital angular momentum off to the atom, but no linear momentum in the axial or radial directions. The selection rules for transitions between different states of the center-of-mass motion of the cold atoms then allow the two fields to couple two rotational states with  $\Delta p = 1$  [22]. For the rotational transitions to be resolvable we need to meet the condition in Eq. (28). This can be arranged to give the following criterion for the detuning

$$\left| \frac{\Delta}{\Gamma} \right| > (k_L w_0)^2 \left| \frac{U_{\min}}{E_R} \right|. \quad (36)$$

For the parameters used above this gives  $\Delta = -4 \times 10^4 \Gamma$ , where  $\Gamma = 9.89$  MHz for Na, in which case our assumed value of  $K = -2 \times 10^5$  corresponds to a laser power of 20  $\mu$ W.

Having calculated the energy spectrum for our two-dimensional artificial molecule, we next consider the feasibility of probing it experimentally. Assuming that atoms can be captured into the annular laser trap in a manner analogous to the loading of laser cooled atoms into tight focus TEM<sub>00</sub> laser traps, it seems reasonable that a relatively large number, of order  $10^3 - 10^4$ , could be trapped [8]. The rotational-vibrational states of the trap might then be probed by pump-probe spectroscopy in a manner similar to the probing of vibrational states in the microscopic traps of optical lattices [25]. Perhaps more promising is a detection scheme developed by Kasevich [26], which probes the atomic motion by inducing stimulated Raman transitions be-

tween states that differ both with respect to center-of-mass and atomic hyperfine ground state. Those atoms that undergo a Raman transition between eigenstates of the center-of-mass motion also change internal states and therefore can be detected with near-unit quantum efficiency. This very high efficiency in detecting transitions between the rotational-vibrational states is necessary because, if one assumes that atoms can be loaded into our annular trap subject to the same restriction as the usual tight-focus traps, then the density of rotational-vibrational states is high enough to render the mean population of any state much less than one. A separate problem is that anharmonicity and rotational-vibrational coupling, together with inhomogeneous broadening from variation in  $w_0$  along the beam axis, will tend to broaden resonances in the pump-probe spectrum.

#### 4. Two-dimensional rotator

In this section we consider the ideal limit in which the cold atoms can be confined to their ground vibrational level. We may then approximate the wave function for the ground electronic state as

$$\psi_g(R, \theta, t) \approx v_{00}(R)\Psi(\theta, t)e^{-iE_{00}t/\hbar}, \quad (37)$$

where  $v_{00}(R)$  and  $E_{00}$  are the ground state eigensolution and associated energy eigenvalue. Substituting in Eq. (20) and projecting with respect to  $v_{00}(R)$  yields the following equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2I} \frac{\partial^2 \Psi}{\partial \theta^2}, \quad (38)$$

where the moment of inertia  $I = MR_{\min}^2$ , and we set  $\chi_q = 1$  for the ground vibrational state. This equation is easily recognized as that for a two-dimensional planar rotator, with eigensolutions  $\psi(\theta, t) = (2\pi)^{-1/2} e^{i(p\theta - E_p t/\hbar)}$ , and energy eigenvalues  $E_p = \hbar^2 p^2 / 2I$ .

Silverman has given an extensive discussion of the physics of two-dimensional planar rotators, ranging from broken symmetry properties in external fields to their relevance to the issue of fractional statistics [1]. Here we would like to concentrate on one of these topics as an illustration of the novel physics which can be explored with the two-dimensional atomic rotator. In particular, we generalize Eq. (38) to allow

for spatially varying gravitational effects over the rotator [27]. This can be done by introducing an angle  $\Theta$  between the  $Z$ -axis perpendicular to the plane of the rotator and the direction of gravity. The rotator equation then becomes

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2I} \frac{\partial^2 \Psi}{\partial \theta^2} + mgR_{\min} \sin(\Theta) \cos(\theta) \Psi. \quad (39)$$

This equation is completely analogous to that describing the Stark effect for a charged planar rotator in an electric field with the gravitational field playing the role of the electric field [1]. To quantify the types of solution Silverman introduces a dimensionless parameter  $Q$  which is a measure of the gravitational potential energy to rotational energy

$$Q = \frac{2MgR_{\min}}{\hbar^2/2I} |\sin(\Theta)| \\ = (k_L w_0)^2 \frac{MgR_{\min}}{E_R} |\sin(\Theta)|. \quad (40)$$

When  $Q < 1$  the rotational kinetic energy term dominates and the energy spectrum of Eq. (39) is that of a two-dimensional rotator to leading-order, as is the case when  $\Theta = 0$ . When  $Q \gg 1$  gravity dominates and the atoms are drawn down around the potential minimum at  $\theta = \pi$  (closest to the Earth). In this case the spectrum becomes that of a harmonic oscillator as the atoms execute small oscillations around the potential minimum with frequency  $2\pi\nu_G = \sqrt{g|\sin(\Theta)|}/R_{\min}$ . For  $\Theta = \pi/2$  and  $w_0 = 10\lambda_L$  we obtain  $Q = 1300$ , and  $\nu_G = 0.24$  kHz, so that the spectrum will be that of a harmonic oscillator. By varying the angle  $\Theta$  we can clearly go between the two extreme cases for the energy spectrum, and Silverman [1] has described in detail how the spectrum changes between the two extreme limits. Clearly, if the gravitational effects are too large they will excite higher radial vibrational levels, and the rotator approximation will be invalid.

Finally, we mention that this system may be used to study quantum chaos, if, for example, the angle  $\Theta$  between the rotator axis and the direction of gravity is periodically modulated. This follows since the classical limit of Eq. (39) is the simple pendulum equation, which is known to show classical chaos when driven appropriately. Moore et. al. [28] have recently explored quantum chaos using an atom optics realization of a quantum  $\delta$ -kicked rotor, and our system would provide a realization of a driven simple pendulum.

## 5. Summary and conclusions

In conclusion, we have shown that cold atoms trapped in annular shaped light shift potentials have the spectrum of artificial 2D molecules with rotational and vibrational states. These artificial molecules will allow for the experimental investigation of the novel selection rules [22] for transitions between rotational-vibrational states which involve conservation of the total orbital angular momentum of the light and atoms, and this might provide new insight into the concept of orbital angular momentum of light fields [13–18]. In the limit that the atoms are constrained to their ground vibrational state, we have a possible atom optics realization of a rotator which could be used to study the novel physics which arise in 2D systems. In particular, we have demonstrated that the effects of gravity in our 2D rotator are completely analogous to the Stark effect for a charged rotator with an applied electric field. The experimental realization of the 2D atomic rotator will join atomic physics with the physics of 2D systems, and this promises new and exciting developments.

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