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# Comment on “Non-destructive light-shift measurements of single atoms in optical dipole traps”

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The light-shift caused by an optical dipole force trap on a single  $^{87}\text{Rb}$  atom was recently studied by Shih and Chapman [Phys. Rev. A **87**, 063408 (2013)] using a dipole-matrix-element-based approach. A separate study by Neuzner *et al.* [Phys. Rev. A **92**, 053842 (2015)] considered the same system using a polarizability-based approach. We find that the results of these two studies do not agree, which we ascribe to an error in the theoretical part of Shih and Chapman’s paper. We correct this error, offer an alternative formulation for the energy-level shift using the matrix-element-based approach, and find good agreement between our predictions and those obtained with the polarizability-based method. Furthermore, our predictions are in better agreement with Shih and Chapman’s experimental results in comparison to their predictions. In contrast to the polarizability-based method, our formulation can be easily extended to different trapping wavelengths and atomic species.

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There is currently great interest in using the optical dipole force (ODF) for trapping ultra-cold atoms, ranging from experiments on trapping single atoms for quantum information processing [1], [2] to large arrays of atoms in lattices for condensed matter studies [3],[4]. One important issue that arises when using the ODF is that the atomic energy levels experience different energy shifts depending on their quantum numbers. These shifts become more pronounced for deep traps and can give rise to deleterious consequences for some applications, unless the trapping beam is at a so-called magic wavelength [5],[6]. Spectroscopic interrogation of trapped atoms requires a precise knowledge of these differential shifts.

There are two common and equivalent methods for predicting the energy shift (also known as the AC Stark shift) of an atom in an ODF trap, one that relies on knowledge of the AC polarizability at the trap wavelength and another that uses the reduced electric-dipole matrix elements for all atomic transitions. Recently, Neuzner *et al.* [7] studied a single  $^{87}\text{Rb}$  atom in an ODF located near the waist of a cavity injected with a linearly-polarized, focused beam of light at a wavelength of  $1.064\ \mu\text{m}$ . They were provided the value of the AC polarizability for  $^{87}\text{Rb}$  at this wavelength based on state-of-the-art theoretical methods and find good agreement between their experimental measurements and theoretical predictions. One downside of this approach is that a new calculation must be performed to predict the polarizability for different trapping-beam wavelengths.

In an earlier free-space experiment under otherwise identical conditions, Shih and Chapman [8] used the matrix-element-based approach to predict the energy level shifts. We find that Shih and Chapman’s prediction for the energy level shifts do not agree with the pre-

diction of Neuzner *et al.* even for trap depths shallow enough to avoid the nonlinear mixing effects investigated by Neuzner *et al.* that occur when the energy shifts are comparable to the hyperfine splittings.

In this Comment, we provide a different formulation for the energy-level shifts in an ODF trap that uses the reduced electric-dipole matrix elements. Our new approach gives predictions that agree with the results of Neuzner *et al.* and removes some cumbersome notation that we believe gave rise to an error in Shih and Chapman’s work. We note that Shih and Chapman leave out some important definitions and notation conventions in [8], although these are largely addressed in Shih’s dissertation [9], yet the prediction error still persists there. Here, we focus on the energy level shifts for  $^{87}\text{Rb}$  in an ODF trap at a wavelength of  $1.064\ \mu\text{m}$  for comparison to these previous works, but our results are easily generalized to other atoms and trap wavelengths.

The energy level shift for an atom in a state  $|\gamma, F, m_F\rangle$  caused by its coupling to all other states  $|\gamma', F', m_{F'}\rangle$  induced by a far-off-resonance, linearly polarized ODF electromagnetic field is well known [9] and is given by

$$\Delta_{\gamma, F, m_F} = -\frac{I}{2\epsilon_0 c \hbar} \times \sum_{\gamma', F', m_{F'}} \delta_{\gamma' F'; \gamma F} |\langle \gamma, F, m_F | \epsilon r_0 | \gamma', F', m_{F'} \rangle|^2, \quad (1)$$

where  $\gamma$  represents the additional quantum numbers needed to uniquely specify the state and

$$\delta_{\gamma' F'; \gamma F} = \left\{ \frac{1}{\omega_{\gamma' F'; \gamma F} + \omega} + \frac{1}{\omega_{\gamma' F'; \gamma F} - \omega} \right\} \quad (2)$$

is a detuning factor with the property that  $\delta_{\gamma' F'; \gamma F} = -\delta_{\gamma F; \gamma' F'}$ . Here,  $\omega_{\gamma' F'; \gamma F} = \omega_{\gamma' F'} - \omega_{\gamma F}$  is the differ-

ence in the bare (unshifted) frequencies of the states,  $\langle \gamma, F, m_F | e r_0 | \gamma', F', m_{F'} \rangle$  is the electric dipole matrix element appropriate for the case when the linear polarization of the trapping beam is aligned with the quantization axis,  $\omega$  ( $I$ ) is the ODF trapping beam frequency (intensity),  $\epsilon_0$  is the permittivity of free space,  $e$  is the electric charge, and  $c$  is the speed of light in vacuum. It is customary and expedient to express the matrix element in terms of the reduced electric dipole matrix element  $\langle \gamma J || e \vec{r} || \gamma' J' \rangle$  and the associated angular momentum coupling coefficients. Unfortunately, there are two different normalization conventions for the reduced matrix elements, which are used with near equal frequency by the atomic physics community and which likely contributed to the error in [8].

To guide us in a choice for the normalization convention that will reduce possible ambiguity and confusion, we consider the case where there are only two isolated states of the atom  $|\gamma_i, F_i, m_{F_i}\rangle$  and  $|\gamma_j, F_j, m_{F_j}\rangle$ . For this situation, the energy shift of one state due to its interaction with the other should be equal in magnitude and opposite in sign to the shift of the other state. That is,

$$\Delta_{\gamma_i, F_i, m_{F_i}} = -\Delta_{\gamma_j, F_j, m_{F_j}}. \quad (3)$$

We find that the normalization convention adopted by the U.S. National Institute of Standards and Technology (NIST) [10], which tabulates many reduced matrix elements, gives a straightforward way to verify that Eq. 3 is satisfied. Shih and Chapman used the other normalization convention [11], which results in level-degeneracy factors appearing in their expressions. Consequently, one must keep track of which state is higher in energy with respect to the other to properly evaluate the matrix elements.

Following the NIST convention, the matrix elements are given by

$$|\langle \gamma, F, m_F | e r_0 | \gamma', F', m_{F'} \rangle|^2 = d^2 (2F+1)(2F'+1) \times \begin{pmatrix} F & 1 & F' \\ -m_F & 0 & m_{F'} \end{pmatrix}_{3j}^2 \begin{Bmatrix} J & J' & 1 \\ F' & F & I \end{Bmatrix}_{6j}^2, \quad (4)$$

where  $d^2 = |\langle \gamma J || e \vec{r} || \gamma' J' \rangle|^2$ . We emphasize that, with this convention,

$$|\langle \gamma J || e \vec{r} || \gamma' J' \rangle| = |\langle \gamma' J' || e \vec{r} || \gamma J \rangle|. \quad (5)$$

Based on the symmetry of the  $3j$  and  $6j$  symbols with respect to interchanging the states, along with Eq. 5, and the symmetry of the remaining terms in Eqs. 4 and 1, it is straightforward to verify that Eq. 3 is satisfied.

As an aside, we note that it is possible to determine  $d$  from the spontaneous emission rate of a higher energy state  $|u\rangle = |\gamma_u, F_u, m_{F_u}\rangle$  decaying to a lower energy state  $|\ell\rangle = |\gamma_\ell, F_\ell, m_{F_\ell}\rangle$  using the relation (following the NIST convention)

$$A_{u \rightarrow \ell} = \frac{\omega_{u\ell}^3}{3\pi\epsilon_0 \hbar c^3} \frac{d^2}{(2J_u + 1)} \quad (6)$$

in SI units, or

$$A_{u \rightarrow \ell} = \frac{2.02613 \times 10^{18}}{\lambda^3} \frac{d^2}{(2J_u + 1)} \quad (7)$$

with  $A_{u \rightarrow \ell}$  in  $\text{s}^{-1}$ ,  $d$  in atomic units ( $ea_0$ , with  $a_0$  the Bohr radius), and the transition wavelength  $\lambda$  in  $\text{\AA}$  [10]. In these expressions, the degeneracy factor  $J_u$  appears, but it is always taken as the quantum number for the higher-energy state. We advocate keeping the procedure for finding  $d$  from  $A_{u \rightarrow \ell}$  distinct and separate from determining the energy level shifts of Eq. 1 to avoid any misunderstanding of interpretation of  $J_u$  in Eq. 7. Shih and Chapman combined these results (using the normalization convention of [11]), which we believe contributed to their error. We note that Shih is aware of the issue regarding the interpretation of the degeneracy factors [9], but appears to have not properly taken this into account when evaluating the energy-level shifts depicted in Fig. 4 of [8] and Fig. 4 of [9].

To illustrate the points made above, we focus on the shifts experienced by the  $5S_{1/2}F=2$  ground state and the  $5P_{3/2}F=3$  excited state of the atom in the ODF trap. Using the equations presented in Shih *et al.*, we reproduce the energy-level shifts presented in their Fig. 4. The results are tabulated in the first row of Tabs. I and II. Though we reproduce Shih *et al.*'s shifts, we obtain a result that is inconsistent with Eq. 3 when we consider an isolated two-level system consisting of the  $m_F = m_{F'} = 0$  states within these levels, for example. For an intensity of  $5.7 \times 10^9 \text{ W/m}^2$ , we obtain  $\Delta_{5S_{1/2}, 2, 0} = -10.63 \text{ MHz}$  and  $\Delta_{5P_{3/2}, 3, 0} = 13.49 \text{ MHz}$ , clearly violating Eq. 3. We believe this error is due to an incorrect interpretation of the degeneracy factors appearing in Eq. 7. Using our formalism, we predict that  $\Delta_{5S_{1/2}, 2, 0} = -10.61 \text{ MHz}$  and  $\Delta_{5P_{3/2}, 3, 0} = 10.61 \text{ MHz}$ , in agreement with Eq. 3.

Going beyond symmetry arguments, we compare the energy-level shifts predicted by Shih *et al.*, Neuzner *et al.*'s polarizability approach, and our approach using Eqs. 1 and 2, now considering the full interaction of the ODF field with the Rb atom. We find that the ground-state shifts are independent of  $m_F$  and that all three approaches are in reasonable agreement, as seen in Table I. We expect such agreement because the ground state is always the lowest energy state and hence there is no ambiguity regarding the degeneracy factors when evaluating Shih *et al.*'s expressions. For our evaluation of their expressions, we use the reduced matrix elements tabulated in Ref. [8]. For the evaluation of Eq. 1, we use the matrix elements tabulated in Ref. [12] which includes all of the transitions considered in Ref. [8] as well as 4 additional transitions from the  $5S_{1/2}$  level to higher  $P$  states and 8 additional transitions from the  $5P_{3/2}$  level to higher lying  $S$  and  $D$  states. For both approaches, we use the transition wavelengths tabulated in Ref. [13]. We assume the errors in the calculation are dominated by the matrix elements and the polarizabilities, and propagate these through the various expressions. There is no error propagated in our calculation of Shih *et al.*'s equation be-

cause they do not provide errors for the matrix elements used in their calculation. For future reference, it is common to associate a temperature  $T$  with the ground state shift using the relation  $-\hbar\Delta_{5S_{1/2},2,m_F} = k_B T$ . A shift of  $-2\pi(18.14 \text{ MHz})$ , calculated from Shih *et al.*'s expression, corresponds to a temperature of 0.87 mK [14].

TABLE I:  $5S_{1/2}, F = 2$  predicted ground-state shift in MHz for  $I = 5.7 \times 10^9 \text{ W/m}^2$  (0.87 mK deep trap).

Shih <i>et al.</i>	-18.14
Neuzner <i>et al.</i>	-18.36(1)
Eqs. 1 and 2	-18.13(4)

While the ground state energy-level shifts are comparable between all three approaches, there is significant disagreement between Shih and Chapman's method and the other two when predicting the shifts of the  $5P_{3/2}$  excited states, as shown in Table II. As explained above, this is due to the misinterpretation of the degeneracy factors.

TABLE II:  $5P_{3/2}, F = 3$  predicted excited-state shifts in MHz for  $I = 5.7 \times 10^9 \text{ W/m}^2$  (0.87 mK deep trap).

	$m_F$			
	0	1	2	3
Shih <i>et al.</i>	53.0	48.9	36.4	15.7
Neuzner <i>et al.</i>	41.5(4)	38.6(4)	29.8(4)	15.0(4)
Eqs. 1 and 2	42.46(6)	39.50(5)	30.62(4)	15.81(4)

Finally, we compare our calculations to Shih and Chapman's experimental measurement of the tuning rate of the  $5S_{1/2}, F = 2 \rightarrow 5P_{3/2}, F = 3$ ,  $\pi$ -polarized transitions as a function of the ODF trap depth. Their data is presented in Fig. 3 of Ref. [8]. Experimentally, the resonance is broadened so much that Shih and Chapman do not resolve the different transition frequencies predicted by all of the theories, although they see substantially larger broadening of the fluorescence signal for the highest trap depths, which could indicate a frequency spread or it could indicate increased atomic motion as they mention. Such broadening makes exact comparison to theory difficult; in the experiment, they measure the centroid of the resonance fluorescence feature as a function of trap depth and find a tuning rate of  $67 \pm 2 \text{ MHz/mK}$ . In Ta-

ble III, we compare this measured tuning rate with the individual transition shifts calculated from the theories described above by determining the differential energy-level shifts at a trap depth of 1 mK. Rows 1, 3, and 4 are the results when we evaluate Shih and Chapman's expressions, Neuzner *et al.*'s expressions, and our expressions, respectively. Shih *et al.* also state their predicted tuning rate for each transition, which is given in Row 2. We are uncertain of the origin of the small difference between Rows 1 and 2, but it does not affect our conclusions.

To compare between the tuning rate measured from the resonance centroid and the theoretical predictions, we note that the fluorescence signal is likely dominated by the  $m_F = 0$  and  $m_F = 1$  transitions because their strength is nearly a factor of two larger than the  $m_F = 2$  transition and hence the tuning rate is more heavily weighted towards these transitions. Shih makes a similar argument in his thesis [9]. Under this assumption, the experimentally measured tuning rate of  $67 \pm 2 \text{ MHz/mK}$  is more consistent with the predictions of Neuzner *et al.*'s and our approaches than with Shih *et al.*'s, consistent with our other findings described above.

TABLE III:  $5S_{1/2}, F = 2 \leftrightarrow 5P_{3/2}, F = 3$   $\pi$ -polarized transition tuning rates in MHz/mK.

	$m_F$		
	0	1	2
Shih <i>et al.</i>	81.8	77.1	62.7
Shih <i>et al.</i> stated	79	74	60
Neuzner <i>et al.</i>	68.8(5)	65.4(5)	55.3(5)
Eqs. 1 and 2	69.6(7)	66.2(6)	56.0(5)

In conclusion, we investigate the disagreement between the results presented by Neuzner *et al.* [7] and Shih and Chapman [8] regarding the energy-level shifts of a single cooled and trapped rubidium atom in an ODF. We identify an apparent error in Ref. [8] and correct it by introducing a new approach that avoids possible ambiguities resulting from level-degeneracy factors. Our approach agrees with the results of Neuzner *et al.* [7] and the experimental data of Shih and Chapman [8]. Unlike the polarizability-based approach used in Ref. [7], our formulation can be extended in a straightforward manner to different atomic species and trapping wavelengths.

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  - [14] Note that Shih and Chapman report a shift of -18 MHz in the caption of Fig. 4 in Ref. [8], which they equate with a trap depth of 0.88 mK. We find that a shift of 18 MHz is equivalent to a 0.86 mK trap depth. On the other hand, when we use their expression for the energy-level shift, we find that it is equal to  $-2\pi(18.14 \text{ MHz})$  or 0.87 mK. We cannot explain these discrepancies with the available information, but these small difference do not change our arguments presented in this Comment.