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Cavity QED level shifts of simple atoms

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We have made a quantitative study of quantum electrodynamic corrections to the energy of some simple atoms near a metallic surface. (i) The two-level atom provides a basic framework within which we discuss the van der Waals, Casimir, and resonant radiative level shifts. In this discussion we show that the level shifts of an excited atom are substantially different from those of a classical dipole antenna. (ii) We calculate the possible cavity QED corrections to the $n=2$ and $n=1$ hydrogen Lamb-shift measurements and obtain results that disagree with the published literature. (iii) We find a general expression for the shifts of the lowest S and P levels of alkali-metal atoms near a conducting surface. These might be studied in the laboratory as a test of cavity QED.

I. INTRODUCTION

Over the past few years there has been a rapid growth of interest in the behavior of atoms confined within cavities of micrometer dimensions. This topic is important both for its connection with basic questions in quantum physics [cavity QED (Refs. 1–3)] and for its practical applications to microelectronic devices such as diode lasers.[4]

From the rather different perspective of ultrahigh-precision spectroscopy and metrology, the level shifts due to cavity QED interactions are a potentially troublesome source of systematic error. This point has been discussed at some length in connection with microwave measurements of the electron g factor.[5] Since recent advances in laser stabilization techniques have made it possible to approach linewidths of 1 Hz at optical frequencies, it seems timely now to extend the discussion to atomic systems such as hydrogen or trapped ions in which very narrow transitions are contemplated.

This paper concerns the shift of atomic energy levels due to the presence of the cavity boundaries, a central aspect of the atom-cavity interaction. The desire to explore these interactions has stimulated efforts both in our laboratory and elsewhere to observe the level shifts of atoms at micrometer distances from a metallic surface. Here we have set about quantifying the magnitude of the shifts and the range over which they may be observed. In order to be specific, we consider the simplest "cavity" boundary: an infinite plane conducting mirror surface. Of course, the infinite plane mirror discussed here is not a particularly close approximation to the sundry pieces of metal that might be present in a typical experimental apparatus, but as we shall see it is quite suitable for discussing the main physical features of the generic problem.

The level shifts are computed here using perturbation theory to order e^2 in the atom-field coupling. Although the perturbative approach is unsuitable for cavities of very high quality factor,[6] it does provide a good approximation in this nonresonant problem.[3] Our starting point is the expression obtained using nonrelativistic quantum electrodynamics for the radiative shift δ_a of atomic energy level a due to the presence of a plane perfect conductor:[7,8]

$$\begin{aligned}\delta_a = &-\sum_{j_>} \frac{k_{aj}^3}{4\pi\epsilon_0}\left(2|\langle a|d_z|j\rangle|^2 U_{aj}^z + |\langle a|d_\rho|j\rangle|^2 U_{aj}^\rho\right)\\ &+\sum_{j_<} \frac{k_{aj}^3}{4\pi\epsilon_0}\left[2|\langle a|d_z|j\rangle|^2 (U_{aj}^z+V_{aj}^z)\right.\\ &\qquad\left.+|\langle a|d_\rho|j\rangle|^2 (U_{aj}^\rho+V_{aj}^\rho)\right] . \end{aligned} \tag{1}$$

The two sums are over higher-lying and lower-lying levels, respectively, and the quantities d_ρ and d_z are the components of the dipole operator parallel and normal to the mirror. The wave vector k_{aj} is defined as $|E_a-E_j|/\hbar c$, E_a and E_j being the unperturbed energies of the levels a and j. The dependence of the level shift upon the distance between the atom and the mirror is contained in the U and V functions defined below:

$$\begin{aligned} U_{aj}^z &= \frac{1}{\pi}\left[\frac{f(\phi_{aj})}{\phi_{aj}^3}+\frac{g(\phi_{aj})}{\phi_{aj}^2}\right] ,\\ U_{aj}^\rho &= \frac{1}{\pi}\left[\frac{f(\phi_{aj})}{\phi_{aj}^3}+\frac{g(\phi_{aj})+1}{\phi_{aj}^2}-\frac{f(\phi_{aj})}{\phi_{aj}}\right] , \end{aligned} \tag{2a}$$

$$\begin{aligned} V_{aj}^z &= \left[-\frac{\cos\phi_{aj}}{\phi_{aj}^3}-\frac{\sin\phi_{aj}}{\phi_{aj}^2}\right] ,\\ V_{aj}^\rho &= \left[-\frac{\cos\phi_{aj}}{\phi_{aj}^3}-\frac{\sin\phi_{aj}}{\phi_{aj}^2}+\frac{\cos\phi_{aj}}{\phi_{aj}}\right] , \end{aligned} \tag{2b}$$

where $\phi_{aj}=2k_{aj}z$ and z is the atom-mirror distance. The functions f and g can be expressed[9] as integrals:

$$f(x)=\int_0^\infty \frac{e^{-xt}}{1+t^2}dt,\quad g(x)=\int_0^\infty \frac{te^{-xt}}{1+t^2}dt . \tag{3}$$

Equation (1) is based on the dipole approximation for the atom-mirror interaction and applies therefore only to atoms that are many diameters away from the surface. At these distances, the very high frequency portion of the vacuum spectrum is not modified significantly by the presence of the mirror and a nonrelativistic approach is quite satisfactory.[10]

Three simple, recognizable, interaction potentials emerge as limiting cases of Eq. (1). They are the van der Waals, Casimir, and resonant radiative interactions.[7,8,11] These limits of the general form are developed in Sec. II for the case of an ideal two-level atom. In addition we give numerical results which are useful in applications to real atoms and we remark upon an interesting failure of the common analogy between an excited atom and a classical dipole antenna.

Section III is a quantitative assessment of cavity QED corrections to high-precision measurements of the Lamb shift.[12,13] Finally, in Sec. IV, we discuss the shifts of the resonance lines of an alkali-metal atom near an ideal conducting surface and compute specific results for sodium and rubidium.

II. TWO-LEVEL ATOM

Many useful insights can be gained from considering a fictitious two-level atom whose levels we label g (ground) and e (excited). Note that the free-space decay rates for parallel (ρ) and normal (z) dipoles are $\Gamma_{\rho,z}=k^3|\langle g|d_{\rho,z}|e\rangle|^2/(3\pi\epsilon_0\hbar)$. Hence the ground-state level shift given by Eq. (1) may be written as

$$\delta_g=-\frac{3\hbar}{4}(2\Gamma_z U^z+\Gamma_\rho U^\rho) , \tag{4}$$

while the excited state shift is

$$\delta_e=\frac{3\hbar}{4}[2\Gamma_z(U^z+V^z)+\Gamma_\rho(U^\rho+V^\rho)] . \tag{5}$$

When the atom is near ($\phi \ll 1$) or far ($\phi \gg 1$) from the mirror, the U and V functions have the particularly simple forms given in Table I. From an experimental viewpoint, the natural questions are the following: (i) over what regions are the near and far approximations valid? and (ii) how does the shift behave in the intermediate region? In order to provide answers to these questions we have evaluated the U functions numerically to determine the exact energy-level shifts at a variety of distances for the two-level atom.

TABLE I. Near- and far-field limits of the U and V functions.

	U^z	U^ρ	V^z	V^ρ
Near: $\phi=2kz \ll 1$	$\frac{1}{2\phi^3}$	$\frac{1}{2\phi^3}$	$-\frac{1}{\phi^3}$	$-\frac{1}{\phi^3}$
Far: $\phi=2kz \gg 1$	$\frac{2}{\pi\phi^4}$	$\frac{4}{\pi\phi^4}$	$-\frac{\sin\phi}{\phi^2}$	$\frac{\cos\phi}{\phi}$

A. Ground state

The ground-state shift close to the mirror ($\phi \ll 1$) is given by the near-field limit of Eq. (4):

$$\delta_g(\text{near})=-\frac{3\hbar}{8\phi^3}(2\Gamma_z+\Gamma_\rho) . \tag{6}$$

This is nothing more than the classical van der Waals potential,[14] which is usually written in the form

$$-\frac{2\langle g|d_z^2|g\rangle+\langle g|d_\rho^2|g\rangle}{64\pi\epsilon_0 z^3} .$$

In this limit, the interaction can be understood as that of the atom's fluctuating electric dipole with its own instantaneous electric image in the mirror. At the other extreme, when the atom is far away from the mirror, the ground-state level shift given by Eq. (4) becomes

$$\delta_g(\text{far})=-\frac{3\hbar}{\pi\phi^4}(\Gamma_z+\Gamma_\rho) . \tag{7}$$

This is the Casimir potential[15] more usually written as $-3\hbar c\alpha_{\text{stat}}/(32\pi^2\epsilon_0 z^4)$, where α_{stat} is the static electric polarizability. At this extreme, the shift is most naturally understood[8] as a change in the Stark shift produced by the fluctuating vacuum—i.e., a change in the Bethe contribution to the Lamb shift[16]—resulting from the modified vacuum field distribution in the presence of the mirror.

Figure 1 shows the ground-state level shifts in the two cases, dipole normal and dipole parallel to the mirror, normalized to $\hbar\Gamma_z$ and $\hbar\Gamma_\rho$, respectively. We see at small distances that the shift approaches the $1/z^3$ van der Waals form [Eq. (6)] as shown by a dashed line for the case of a dipole normal to the mirror. At large distances, the level shift becomes independent of the orientation of

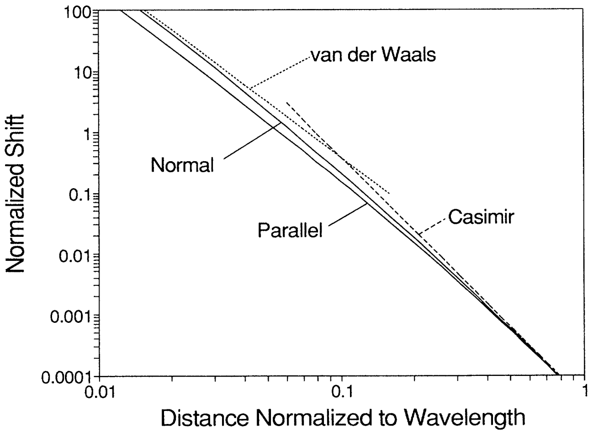

FIG. 1. Cavity QED shifts of the ground-state energy in a two-level atom near a plane mirror. Solid lines show the shifts due to an electric dipole normal (d_z) or parallel (d_ρ) to the mirror. Dashed lines show the van der Waals potential (for d_z) and the Casimir potential which is isotropic. Each shift is normalized to the energy, $\hbar\Gamma_z$ or $\hbar\Gamma_\rho$, associated with that dipole coupling. The distance from the mirror is normalized to the wavelength of the resonant radiation.

the dipole and tends to the $1/z^4$ Casimir form [Eq. (7)] also indicated. In the intermediate region, centered in the vicinity of $\lambda/10$, there is a smooth transition from one form to the other.

Consider now Fig. 2, which displays the ratio of the ground-state level shift to the limiting van der Waals and Casimir potentials. As well as showing the asymptotic behavior, this figure provides quantitative information about the behavior of the potential at intermediate distances. It reveals the remarkably simple result that, within a factor of 2, the van der Waals potential is correct at distances less than 0.12λ while the Casimir potential is correct at longer range.

B. Excited state

In the region close to the mirror, the level shift of the excited state is given by the near-field limit of Eq. (5):

$$\delta_e(\text{near}) = -\frac{3\hbar}{8\phi^3}(2\Gamma_z+\Gamma_\rho)\ . \tag{8}$$

We see that this expression is identical to the van der Waals shift of the lower level [Eq. (6)] and therefore there is no net change in the resonant frequency of this two-level atom. Real atoms, of course, have more than two levels and their resonances do not exhibit this fortuitous cancellation.[7]

At large distances, the excited-state level shift [Eq. (5)] is dominated by the oscillatory V terms which are absent from the ground-state shift:

$$\delta_e(\text{far}) = -\frac{3\hbar}{4}\left[\frac{2\Gamma_z\sin\phi}{\phi^2}-\frac{\Gamma_\rho\cos\phi}{\phi}\right]\ . \tag{9}$$

Figure 3 displays the ground- and excited-state level shifts for the case of a dipole that is parallel to the mirror. For comparison, the van der Waals shift is also indicated.

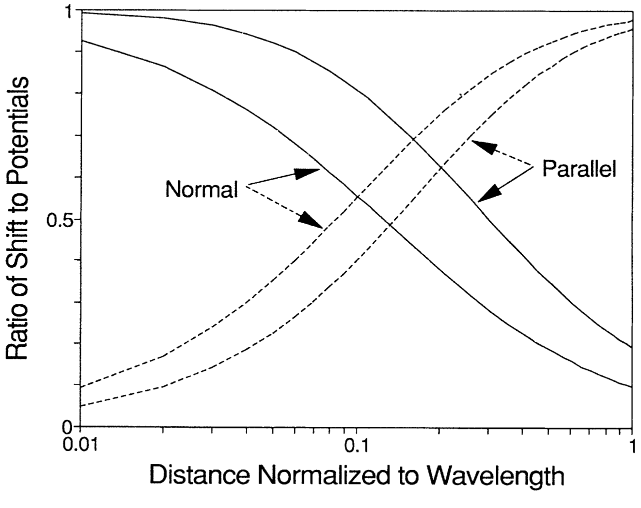

FIG. 2. Ratio of exact ground-state energy shifts in a two-level atom to the van der Waals and Casimir potentials. Solid lines show this ratio for the van der Waals potential and dashed lines for the Casimir potential.

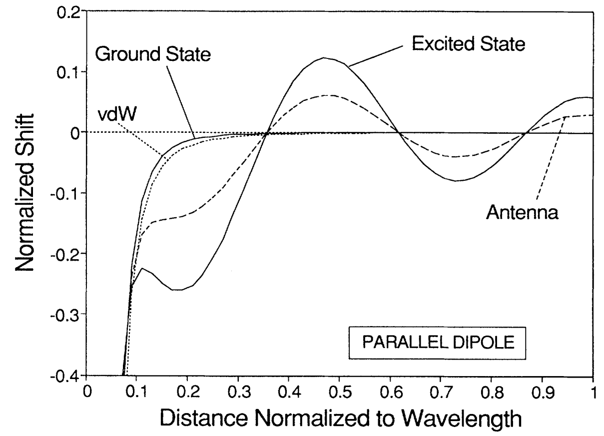

FIG. 3. Solid line: cavity QED energy level shifts in a two-level atom near a plane mirror due to a parallel dipole d_ρ. Dotted line: the van der Waals potential for the atom. Dashed line: interaction energy of a classical antenna with the mirror; the normalization of this curve is discussed in the text.

C. Comparison with classical antenna

It is interesting to make a comparison between the excited-state level shift of Sec. II B, calculated using QED, and the energy ΔW of a classical dipole antenna interacting with its own reflected field.[17] This is

$$\Delta W = \frac{k^3}{8\pi\epsilon_0}(2\overline{d_z^2}V^z+\overline{d_\rho^2}V^\rho)\ , \tag{10}$$

where $\overline{d_{z(\rho)}^2}$ is the mean-square dipole moment of the antenna in the normal (parallel) direction. If we identify the classical average $\overline{d_\mu^2}$ with the quantum-mechanical expectation value $\langle e|d_\mu^2|e\rangle$, the atom and antenna have identical shifts close to the mirror, as shown in Fig. 3, but at large distances, the shift of the antenna is only half that of the atom. If instead we choose to identify $\overline{d_\mu^2}$ with $2\langle e|d_\mu^2|e\rangle$ (as is traditional),[18] the long-distance potentials are reconciled, but now the near-field interactions differ by a factor of 2. This is an interesting result because it shows that the excited two-level atom does not have a simple correspondence with the classical radiator.

We propose a viewpoint which seems to resolve this issue. Meschede, Jhe, and Hinds[8] have shown that only half the far-field shift is due to self-reaction (the remainder being generated by the vacuum fluctuations), whereas the near-field van der Waals shifts appears as a pure self-reaction effect, fully analogous to the classical antenna. This suggests to us that the far-field shift of the antenna should indeed be only half that of the corresponding atom and we are led, against tradition, to associate $\overline{d_\mu^2}$ with $\langle e|d_\mu^2|e\rangle$. It is well known that with this correspondence, the power radiated from an antenna in free space is only half that of the atom.[18] However, this is also acceptable since Dalibard, Dupont-Roc, and Cohen-Tannoudji[19] have shown that only half the power radiated from an atom does correspond to a classical

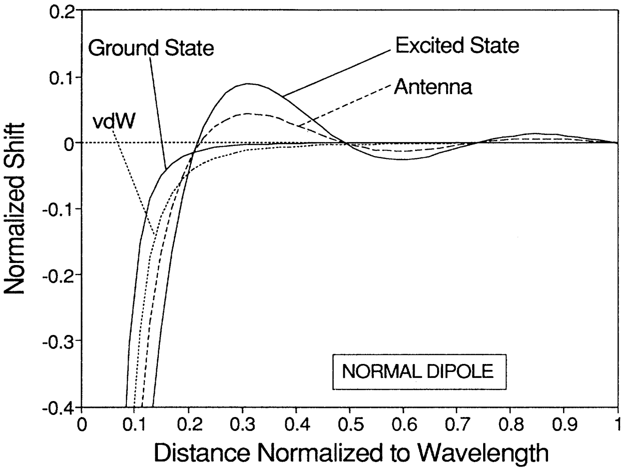

FIG. 4. Energy shifts as in Fig. 3, but for the case of a dipole normal to the mirror.

self-reaction effect. The most obvious experimental test of this difference between atom and antenna is simply to compare their near-field and far-field shifts.

Figure 3 clearly shows that the large oscillating shift of the excited state greatly exceeds the ground-state shift as Barton has previously emphasized.[20] The corresponding plot for a normal dipole, Fig. 4, shows similar general features although the long-range shift is smaller in this case because the dipole cannot launch a free radiation field in the direction normal to the mirror.

In precision measurements of atomic intervals it is usual to keep the atoms away from surfaces because of the risk of level shifts due to stray electric fields. Any systematic errors due to cavity QED level shifts are therefore likely to be dominated by the oscillatory far-field interactions. Since these level shifts are proportional to the radiation rate, a spectral line of small natural width is less susceptible to cavity QED shifts than a broad one. Of course, a narrow line is desirable in precision measurements for numerous other reasons as well.

III. CORRECTIONS TO THE HYDROGEN LAMB SHIFT

Metastable atomic hydrogen is a rather unsuitable system for the study of cavity effects because it is inconvenient to produce and is easily quenched by modest electric fields. Indeed, to date, experiments to study cavity QED have used more convenient atoms. On the other hand, extremely high-precision measurements have been made of the $2S_{1/2}$-$2P_{1/2}$ Lamb shift in hydrogen.[13] Since these provide a stringent test of bound-state QED, it is of interest to assess the systematic corrections that might be required to account for unwanted cavity QED perturbations.[21]

A. The $2S_{1/2}$ level

The spectrum of electric dipole transitions involving the $2S$ multiplet has two very long wavelength components (30 and 3 cm) connecting it to $2P_{1/2}$ and $2P_{3/2}$. On this scale, we assume a short distance from the atom to the surface so that the $2P$ levels contribute shifts of the van der Waals type (Table I) to the total shift of $2S$. In any hyperfine sublevel μ of the $2S$ multiplet this $2P$ contribution to the total shift is

$$\delta^{2P}_{2S,\mu}=\frac{-1}{64\pi\epsilon_0 z^3}\sum_{\gamma} 2|\langle 2S,\mu|d_z|2P,\gamma\rangle|^2 + |\langle 2S,\mu|d_\rho|2P,\gamma\rangle|^2 , \tag{11}$$

where the sum is over all the $2P$ fine and hyperfine sublevels γ. The result is a scalar shift, independent of the particular state μ. This is not surprising, for the van der Waals interaction transforms under coordinate-space rotations as a combination of scalar and rank-two tensor which can only produce a scalar shift in S states. The remaining levels that contribute to the shift all lie above $2S$ and involve wavelengths that are 656 nm or less. Assuming that the atom-mirror distance is much greater than 65 nm ($z \gg \lambda/10$), these levels cause scalar shifts of the Casimir type:

$$\delta^{nP}_{2S,\mu}=\sum_{n=3}^{\infty}\sum_{\gamma}\left[\frac{-k^3}{\pi^2\epsilon_0\phi^4}\right]_{2S,nP}(|\langle 2S,\mu|d_z|nP,\gamma\rangle|^2 + |\langle 2S,\mu|d_\rho|nP,\gamma\rangle|^2) , \tag{12}$$

After some algebra, one finds that the entire shift in a $2S$ state is

$$\delta_{2S}=-\frac{e^2}{4\pi\epsilon_0}\left[\left[\frac{R^2}{12z^3}\right]_{2S,2P}+\sum_{n=3}^{\infty}\left[\frac{R^2}{4\pi k z^4}\right]_{2S,nP}\right] , \tag{13}$$

where R indicates the radial integral and k is the wave vector for each $2S$-nP interval. This is not a large shift; for instance, even at a distance as small as 1 μm it amounts only to -2.3 kHz.

B. The $2P_{1/2}$ level

Similarly, the $2P_{1/2}$ level has a van der Waals coupling with $2S_{1/2}$ and Casimir couplings to the higher S states. For example, at 1 μm from the surface these interactions together shift the $2P_{1/2}$ level by -0.8 kHz. In addition, however, $2P_{1/2}$ has a strong radiative dipole coupling to the ground state which produces the much larger long-range oscillatory shift given by the V terms of Eq. (5) as described in Sec. II B above. This can be viewed as the result of the reabsorption of reflected spontaneous Lyman-α (121 nm) radiation. If we assume (rather artificially) that the mirror is a perfect reflector at that wavelength, and if we continue to assume that the distance from the mirror is much larger than 65 nm, then $\phi_{2P,1S} \gg 1$ and this resonant radiative shift is given to a good approximation by

$$\delta_{2P_{1/2}}=\frac{\hbar}{2}\left[\Gamma\frac{\cos\phi}{\phi}\right]_{2P,1S} , \tag{14}$$

where Γ is the $2P$ decay rate. At a distance of 1 μm from the surface, the amplitude of this oscillatory shift is approximately 500 kHz and it completely dominates the total $2P_{1/2}$ level shift. Moreover, since it decreases with distance as $1/z$, this term dominates the level shift at all larger distances.

C. Discussion

Our view of the $2S_{1/2}$ and $2P_{1/2}$ level shifts is in striking disagreement with that of Cheon,[21] who considered the shifts of these same levels when the hydrogen atom is placed between two plane parallel mirrors separated by 1 μm. Naturally, the one- and two-mirror shifts should differ, but only in relatively minor numerical factors.[3] The main discrepancy is that Cheon finds no shift of $2P_{1/2}$ and a −894-kHz shift of $2S_{1/2}$, whereas we find a large (∼500-kHz) oscillating shift of $2P_{1/2}$ and a very small (∼−2-kHz) $2S_{1/2}$ shift. Since our starting point [Eq. (1)] has been derived by several different authors,[7,8,11] we believe that the result of Cheon is in error.

Of course, Lamb-shift experiments are not conducted at a distance of 1 μm from a mirror. We presume that in any such measurement, the hydrogen is at least 1 mm away from reflecting surfaces. Then the $2S_{1/2}$ shift is negligible (μHz) while the oscillating $2P_{1/2}$ shift is no greater than 500 Hz—less than 10% of current experimental accuracy. Furthermore, the net effect should be substantially less when averaged over the rapid $\cos\phi$ oscillations. We conclude, therefore, that the existing Lamb-shift measurements require no cavity QED correction.

Future experiments are more likely to focus on the narrow $1S$-$2S$ two-photon uv laser transition which may eventually be used to determine the ground-state Lamb shift at the 1-Hz level of accuracy. As we have noted at the end of Sec. II C, lines of narrow natural width are particularly insensitive to far-field cavity QED shifts. Our conclusion is again in disagreement with that implied by the work of Cheon: we believe that in this case the cavity QED shifts should be much less than 1 Hz and would introduce no significant error.

IV. ALKALI-METAL RESONANCE LINES NEAR A SURFACE

Our last computation concerns the shifts of the alkali-metal resonance lines near a surface. After some angular momentum algebra, Eq. (1) leads to the following shifts for the lowest S and P levels of sodium:

$$\delta_{3S_{1/2}} = -\sum_{n=3}^{\infty} \frac{3\hbar}{2}[A(U^z+U^\rho)]_{nP,3S} , \tag{15}$$

$$\begin{aligned}\delta_{3P_{1/2}} = &-\sum_{n=4}^{\infty} \frac{\hbar}{6}[A(U^z+U^\rho)]_{nS,3P} \\ &-\sum_{n=3}^{\infty} \frac{5\hbar}{6}[A(U^z+U^\rho)]_{nD,3P} \\ &+\frac{\hbar}{2}[A(U^z+V^z+U^\rho+V^\rho)]_{3P,3S} ,\end{aligned} \tag{16}$$

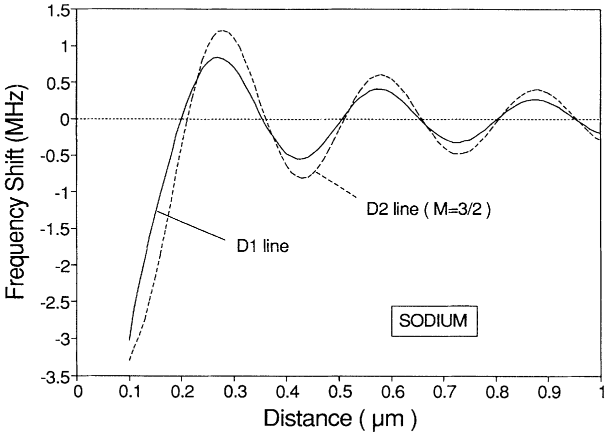

FIG. 5. Frequency shifts of the sodium D lines vs distance of the atom from a plane perfect mirror.

$$\begin{aligned}\delta_{3P_{3/2},|M_J|=3/2} = &-\sum_{n=4}^{\infty} \frac{\hbar}{4}[A(U^\rho)]_{nS,3P} \\ &-\sum_{n=3}^{\infty} \frac{\hbar}{8}[A(6U^z+7U^\rho)]_{nD,3P} \\ &+\frac{3\hbar}{4}[A(U^\rho+V^\rho)]_{3P,3S} ,\end{aligned} \tag{17}$$

$$\begin{aligned}\delta_{3P_{3/2},|M_J|=1/2} = &-\sum_{n=4}^{\infty} \frac{\hbar}{12}[A(4U^z+U^\rho)]_{nS,3P} \\ &-\sum_{n=3}^{\infty} \frac{\hbar}{24}[(22U^z+19U^\rho)]_{nD,3P} \\ &+\frac{\hbar}{4}\{A[4(U^z+V^z)+U^\rho+V^\rho]\}_{3P,3S} ,\end{aligned} \tag{18}$$

where A is the Einstein coefficient for the transition and U and V are the functions defined by Eqs. (2) and (3). All

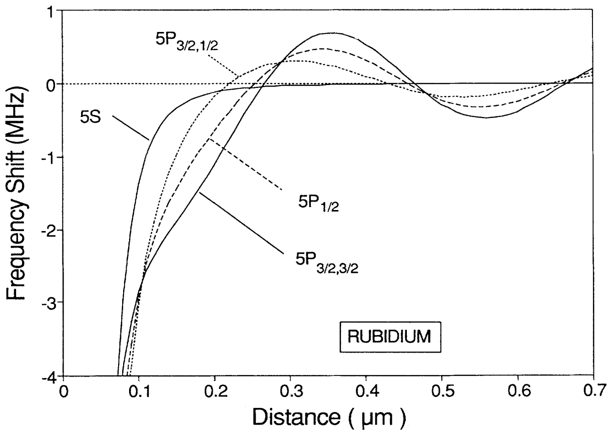

FIG. 6. Energy-level shifts (divided by Planck's constant) in the lowest S and P states of rubidium.

three of these quantities depend on the particular pair of configurations $nl,n'l'$ and must therefore be reevaluated for each term in the sums above (we ignore the small effects of fine structure on the wavelengths and the radial integrals).

Figure 5 shows the frequency shifts of the $D1$ and $D2$ lines of sodium near a conducting surface as given by Eqs. (15)–(17). The large oscillations at long range are precisely those of the two-level atom ($3S$ and $3P$ in this case). Closer to the mirror, the shift evolves into a $1/z^3$ form which is due to the difference between the van der Waals shifts of the $3S$ and $3P$ levels. The ground-state van der Waals shift is virtually all due to the same two-level ($3S$-$3P$) coupling, but the $3P$ level is significantly shifted by $3D$, $4D$, and $4S$ as well as by $3S$. Since these significant couplings involve only a few wavelengths in the range 590–1697 nm, the validity of the theoretical results depends only on having a high reflectivity at those wavelengths and our assumption of an ideal mirror is not, in fact, very restrictive.

The hyperfine lines within the $D1$ multiplet are all equally shifted because this is an electric interaction which cannot distinguish between $m_J=+\frac{1}{2}$ and $-\frac{1}{2}$. This is not the case in the $D2$ lines since the $3P_{3/2}$ level shift is a tensor, but we nevertheless continue to ignore the hyperfine structure here in the interests of simplicity.

Although Eqs. (15)–(18) apply to sodium, they can also be used for any other alkali metal with nothing more than a change of the principal quantum numbers. These formulas should therefore be of general use in the interpretation of alkali-metal spectra taken close to a surface. As a further example we show the rubidium level shifts (Fig. 6). There is some experimental evidence for such shifts in cesium.[22]

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