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Quasi orbital motion of ultra cold excited atomic dipole near dielectric microsphere

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Abstract. We consider the dynamics of the center-of-mass of an ultracold excited atomic oscillator in the vicinity of a dielectric microsphere. The specific parameters of microsphere (dielectric constant, radius) allowing for atom's quasi orbital motion, with an arbitrary orientation of dipole momentum, are analyzed. We discuss the conditions for which excited atoms like alkalis, alkaline earths or noble gases could form a kind of atom-microsphere exciplex with different orbital momenta.

PACS. 32.80.Lg Mechanical effects of light on atoms, molecules, and ions – 34.50.Dy Interactions of atoms, molecules, and their ions with surfaces; photon and electron emission; neutralization of ions – 42.25.Gy Edge and boundary effects; reflection and refraction

An interesting example of atomic motion around a dielectric microsphere ("atom galleries") was proposed in [1]. This motion is possible for a three-level atom near a dielectric microsphere with external two-frequency excitation. The atom motion in this case is similar to the motion of the Earth around the Sun.

In the present paper, we consider another type of quasi-orbital motion, *without* external fields. This quasi-orbital motion, driven by Whispering Gallery Modes (WGM) *vacuum* field, is possible for a two-level excited atom, with arbitrary orientation of dipole momentum, near a dielectric microsphere [2]. The geometry of the problem is given in Figure 1.

The existence of a quasi-orbital motion is determined by the topology of atom-microsphere interaction potential, which is proportional to level shift or frequency shift. That is why one should find the conditions which provide the necessary space topology of frequency shifts.

Let us consider an atom with fixed orientation of dipole momentum. The quasi-orbital motion of such an atom in radial direction is quite possible. Indeed, as shown in [2–4], the dependence of atomic frequency shifts on the distance from microsphere surface exhibits the characteristic oscillations due to interaction with freely-propagating radiation reflected by microsphere. Consequently this dependence has minima, which are suitable for quasi-orbital motion.

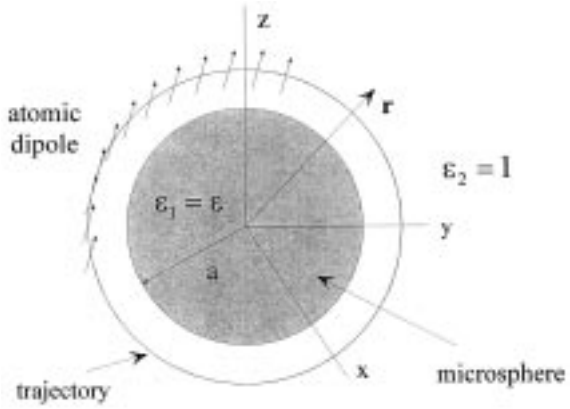

Fig. 1. Geometry of the problem.

However such a simple approach cannot be used to trap an atomic oscillator with an arbitrary orientation of dipole momentum. This is due to the fact that the energy minima positions for different dipole orientations do not coincide. Moreover, the situation appears more complicated when we take into account the center-of-mass motion of the atomic oscillator. The reason is that a radially oscillating atom acquires tangential components when orbiting around the microsphere surface, and *vice versa* due to pure kinematic reasons. Hence, if one tunes the parameters for radial dipole orientation, the atom revolution along one quarter of circle changes the dipole orientation to a tangential one for which, in general, the potential energy minimum is not located at the same distance.

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$$\left(\frac{\omega-\omega_0}{\gamma_0}\right) = -\frac{3}{4}\mathrm{Im}\Big[\cos^2\psi\sum_{n=1}^{\infty} n(n+1)(2n+1)q_n\left(\frac{h_n^{(1)}(z')}{z'}\right)^2 + \sin^2\psi\sum_{n=1}^{\infty}(n+1/2)\left\{p_n(h_n^{(1)}(z'))^2 + q_n\left(\frac{d(z'h_n^{(1)}(z'))}{z'dz'}\right)^2\right\}\Big]. \quad (1)$$

A simpler situation occurs when the dipole orientation is perpendicular to the plane of rotation. In this case the dipole orientation is always tangential.

That is why the potential energy of excited atom should have simultaneous minimum for *arbitrary* orientation of dipole momentum, to allow for a stable quasi-orbital motion around the dielectric microsphere. In the present paper, within classical as well as quantum mechanical approaches, we will show that such a topology can be created by fine tuning of microsphere radius and dielectric constant.

The method of calculation of frequency shift within classical approach was considered in [2] and the perturbative expression for frequency shift of atomic dipole with arbitrary orientation has the form:

see equation (1) above.

Here, ω_0, γ_0 are free-space radiation frequency and line width respectively; ψ is the dipole orientation angle ($\psi = 0$ corresponds to radial orientation); j_n and h_n are spherical Bessel functions [5]; $z' = kr$.

All information about microsphere optical properties is contained in q_n and p_n – Mie reflection coefficients [6]:

$$q_n = \frac{\left[\epsilon\frac{d}{dz_2}[z_2 j_n(z_2)]j_n(z_1) - \frac{d}{dz_1}[z_1 j_n(z_1)]j_n(z_2)\right]}{\left[\epsilon\frac{d}{dz_2}[z_2 h_n^{(1)}(z_2)]j_n(z_1) - \frac{d}{dz_1}[z_1 j_n(z_1)]h_n^{(1)}(z_2)\right]} \quad (2)$$

$$p_n = \frac{\left[\frac{d}{dz_2}[z_2 j_n(z_2)]j_n(z_1) - \frac{d}{dz_1}[z_1 j_n(z_1)]j_n(z_2)\right]}{\left[\frac{d}{dz_2}[z_2 h_n^{(1)}(z_2)]j_n(z_1) - \frac{d}{dz_1}[z_1 j_n(z_1)]h_n^{(1)}(z_2)\right]}. \quad (3)$$

In equations (2, 3) and elsewhere, $z_1 = \sqrt{\epsilon}ka; z_2 = ka$, ($a$: microsphere radius, k: wavenumber in free space).

The quantum mechanical perturbative expression for the frequency shift differs from equation (1) by a non resonant term, which is of importance only in close vicinity to microsphere surface [7]. This quantum mechanical addendum is not likely to influence our result substantially. This influence will be considered elsewhere.

Here we apply equation (1) to find the parameters for quasi-orbital motion of an atomic oscillator with arbitrary orientation of dipole momentum. To do this, we need to consider microspheres with high dielectric constant in the optical region. Microspheres with large dielectric constant are necessary to reduce microsphere radius and consequently the period of atom revolution around microsphere. Here for definiteness, we consider the case of microsphere made of diamond with $\epsilon = 6.01$.

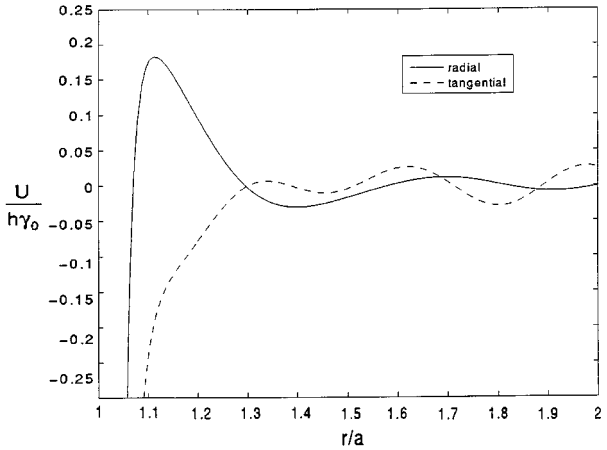


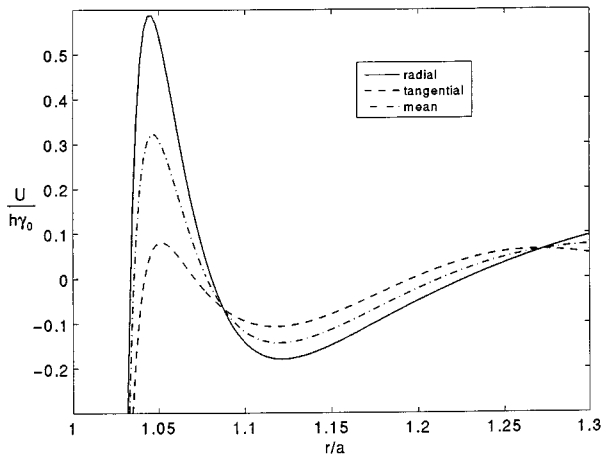
Fig. 2. Relative frequency shift $(\omega - \omega_0)/\gamma_0$ as a function of the position (r/a) of the radially (solid line) and tangentially (dashed line) oscillating atomic dipole near microsphere. General parameter case ($ka = 10.1$ and $\epsilon = 6$).

Figure 2 shows the typical dependence of frequency shift for general system parameters. From this figure one can easily see that, for arbitrary orientations, a quasi-orbital motion is possible very close to the surface due to pure electrostatic (van der Waals-type) forces. However, it is very difficult to put atoms into this region, because of the inevitable capture of atom by microsphere, due to short range attraction singularity. Subsequently we will not consider this trivial case.

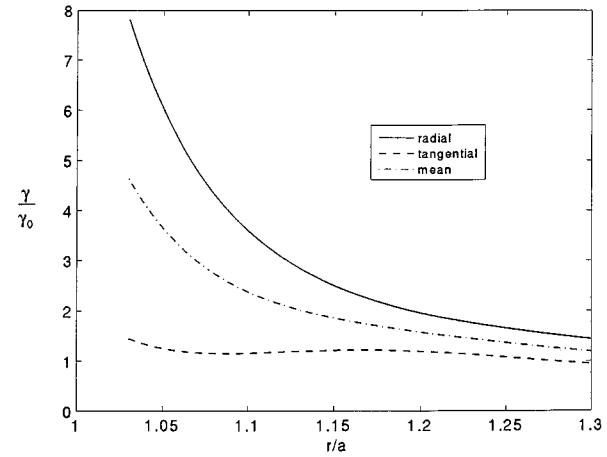
As for the case of large distances, the potential minimum of a radially oriented dipole (at $r = 1.4a$) does not coincide with the positions of the potential minima of a tangentially oriented dipole (at $r = 1.45a, 1.8a$). Hence, the quasi-orbital motion of radially oriented dipole does not result in a quasi-orbital motion of tangentially oriented dipole. Besides, the arbitrary choice of microsphere parameters does not provide the deepest well.

The difficulty in getting quasi-orbital motion is due to the characteristic features of interaction of microsphere eigenmodes with atomic dipole with different orientations. Indeed, according to equation (1), the radially oriented dipole ($\psi = 0$) interacts only with transverse magnetic, TM, modes (Mie coefficients q_n), while the tangentially oriented dipole ($\psi = \pi/2$) interacts with TM modes as well as transverse electric (TE) modes (Mie coefficients p_n). The interaction of tangential dipole with TM-modes makes difficult the determination of the capture parameters because the latter interaction contains derivatives of Bessel functions. If this interaction were absent, the simultaneous maximization of p_n and q_n for some n should give access to a quasi-orbital atomic motion.

$$\frac{U_{eff}}{\hbar\gamma_0} = \left(\frac{\omega-\omega_0}{\gamma_0}\right)_{eff} = -\frac{3}{8}\mathrm{Im}\Big[\sum_{n=1}^{\infty} n(n+1)(2n+1)q_n\left(\frac{h_n^{(1)}(z')}{z'}\right)^2 + \sum_{n=1}^{\infty}(n+1/2)\left\{p_n(h_n^{(1)}(z'))^2 + q_n\left(\frac{d(z'h_n^{(1)}(z'))}{z'dz'}\right)^2\right\}\Big]. \quad (6)$$



(a)



(b)

Fig. 3. Relative frequency shift $(\omega-\omega_0)/\gamma_0$ (a) and line width γ/γ_0 (b) as a function of the position (r/a) of the radially (solid line) and tangentially (dashed line) oscillating atomic dipole near microsphere. Capture parameter case ($ka = 10.488\,95$ and $\epsilon = 6.01$). The dashed-dotted lines show the orientation-averaged frequency shift and linewidth.

Nevertheless the direct numerical simulation allows us to find a number of specific (non resonant!) values of microsphere radius at which the positions of radial and tangential wells will be close.

In Figure 3 one can see a special situation ($ka = (ka)^* = 10.488\,95, \epsilon = 6.01$) which results in a quasi-orbital motion of the atom near $r = 1.125a$.

The dependence of related Mie reflection coefficients (Eqs. (2, 3)) and atomic oscillator line on ka is shown in Figure 4. Let us identify the whispering gallery modes (TM and TE) by the triple number (P, n, m), where P characterizes the number of zeros of $j_n(\sqrt{\epsilon}kr)$ inside the microsphere ($P = 1$ – no zero, $P = 2$ – one zero, *etc.*); n and m characterize the orbital and azimuthal quantum numbers respectively. One may see from Figure 4 that the atomic oscillator frequency is out of strong WGM resonances, and the perturbation theory is valid in this region. The TM (1, 20, 20) resonance ensures the potential barrier between atom and microsphere surface.

Let us consider the properties of this quasi-orbital motion in more detail (Fig. 3). In the absence of orbital motion of atom, the peak energy of atom is determined by the well depth only. For a radial dipole orientation, we have

$$E_{max} \approx 0.2\hbar\gamma_0 \quad (4)$$

while for a tangential dipole

$$E_{max} \approx 0.3\hbar\gamma_0. \quad (5)$$

The case of orbital motion is more interesting. Below we will show that, in this case, it is possible to capture atom with larger energy.

In the present paper, we will perform a preliminary investigation of quasi-orbital motion of excited atom. To do this, we will use the spherically symmetric expression for the potential. This expression is a result of averaging of equation (1) over atom trajectory around microsphere. Averaging over trajectory is equivalent to averaging over dipole orientation which can be performed easily within the framework of equation (1).

For the case of dipole momentum lying in the plane of rotation, the spherically symmetric expression for effective potential becomes:

see equation (6) above.

Expression (6) is shown in Figure 3 by dashed-dotted line. The radial motion of atom is described by the potential [8]:

$$U(r) = U_{cf}(r) + U_{eff}(r) = \frac{M^2}{2mr^2} + U_{eff}(r). \quad (7)$$

Here $M = mVr$ is the orbital momentum (V: azimuthal velocity, m: atom mass).

The dependence of potential (Eq. (7)) on the orbital momentum is shown in Figure 5.

The peak orbital momentum (and azimuthal velocity) is defined by the condition of disappearance of the minimum of equation (7). In our case ($ka = (ka)^* = 10.488\,95$, $\epsilon = 6.01$), we have

$$\frac{M^2}{2ma^2\hbar\gamma_0} = \xi^* \approx 1.5. \quad (8)$$

Table 1. Fraction of revolution for some commonly used atoms.

Atom	Mass	Transition	λ (nm)	τ (ns)	Fraction of revolution	
					$\epsilon = 6$	$\epsilon = 50$
Mg	24	2^1S_0–2^3P_1	457.1	4.6 ms	1	4.8
Ca	40	3^1S_0–3^3P_1	657.5	0.4 ms	0.2	0.8
Rb	85	$5S_{1/2}$–$5P_{3/2}$	780.0	26.5	0.001	0.004
Xe	131	$6s[3/2]_2$–$6p[5/2]_3$	881.9	34	0.001	0.003
Cs	133	$6S_{1/2}$–$6P_{3/2}$	852.1	30	0.001	0.003

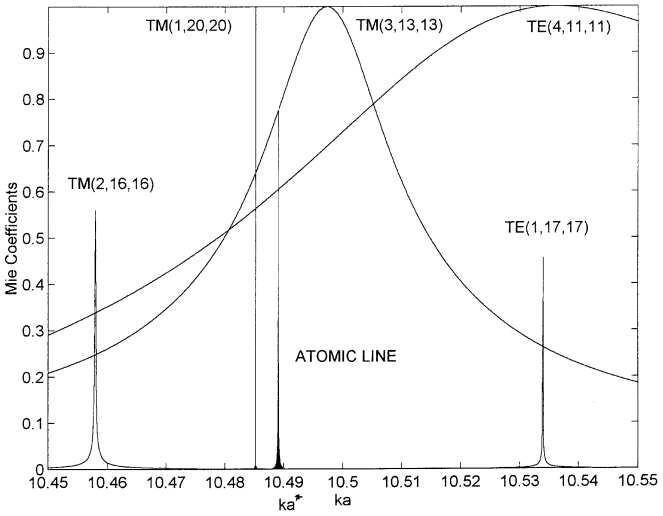


Fig. 4. Dependence of absolute values of the related TM and TE Mie coefficients on ka. The atomic oscillator line for capture case is shown by filled Lorenz curve ($\omega_0/\gamma_0 = 10^5$).

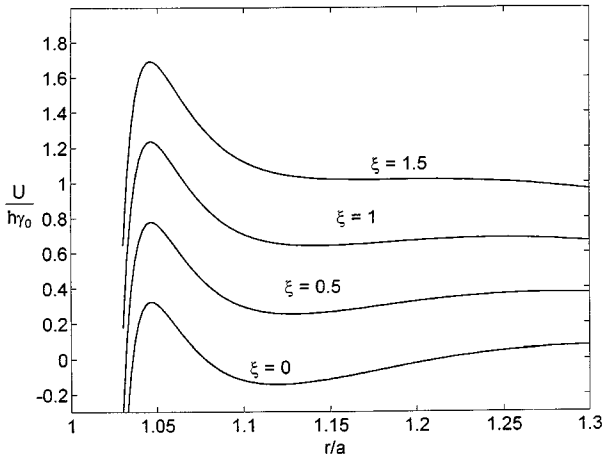


Fig. 5. Dependence of radial potential on orbital momentum ($M^2/2ma^2\hbar\gamma_0 = \xi$; $\xi = 0$, 0.5, 1, 1.5).

In addition, the disappearance of capture takes place at $r^* \approx 1.15a$. One can see easily that it is possible to capture an atom with

$$E_{max} = \frac{\xi^*}{(r^*/a)^2}\hbar\gamma_0 \approx 1.1\hbar\gamma_0. \tag{9}$$

This is a significant increase in comparison with the case of absence of azimuthal motion (see Eqs. (4, 5)).

From equation (8), it is easy to find the atom velocity and rotation period:

$$V \approx \sqrt{\frac{2\xi^*}{\tilde{r}^{*2}}\frac{\hbar\gamma_0}{m}}, \quad T = 2\pi\sqrt{\frac{\tilde{r}^{*4}}{2\xi^*}\frac{ma^2}{\hbar\gamma_0}} \tag{10}$$

where $\tilde{r}^* = r^*/a$, dimensionless radial coordinate of the potential well minimum. To form a circular orbit, the rotation period should be comparable with excited atom lifetime, *i.e.*

$$T \sim 1/\gamma_0 \tag{11}$$

or

$$2\pi\sqrt{\frac{\tilde{r}^{*4}}{2\xi^*}\frac{m\gamma_0 a^2}{\hbar}} \sim 1. \tag{12}$$

It is easy to see that, for sufficiently small transition line width and microsphere radius, this condition always holds.

Note that the microsphere radius cannot be made arbitrarily small, because it is connected with the optical wavelength at which the large dielectric constant exists. Taking this remark into account one can rewrite (12) in the form:

$$\sqrt{\frac{\tilde{r}^{*4}(ka)^{*2}}{2\xi^*}\frac{m\gamma_0\lambda^2}{\hbar}} \sim 1 \tag{13}$$

where $(ka)^*$=10.488 95 – a value derived above for the relation between microsphere radius and free radiation wavelength. Substituting the numbers we obtain the rotation condition which depends only on excited atom characteristics:

$$8\sqrt{\frac{m\gamma_0\lambda^2}{\hbar}} \sim 1. \tag{14}$$

Table 1 shows the number of revolutions for some atomic oscillators (see, for example, [9]) in case under consideration. The analysis of this table shows that the only atom which can perform full revolution is Mg. Note the orbital velocity in this case is about

$$V \approx \sqrt{\frac{\hbar\gamma_0}{m}} \sim 1 \text{ mm/s}. \tag{15}$$

Above, the principle of capture of an excited atom with arbitrary orientation of dipole momentum near dielectric microsphere was demonstrated. Moreover some atomic dipoles (*e.g.*, Mg) can rotate around microsphere.

Up to now we considered purely classical dynamics of the center of mass of the atomic dipole. However if we rewrite equation (13) in the form:

$$2\pi\sqrt{\frac{\tilde{r}^{*4}}{2\xi^*}\frac{ma^2\gamma_0}{\hbar}} = 2\pi\frac{a}{\lambda\!\!\!^{-}}\sqrt{\frac{\tilde{r}^{*6}}{4\xi^{*2}}} \approx \pi\frac{a}{\lambda\!\!\!^{-}} \sim 1 \qquad (16)$$

where $\lambda\!\!\!^{-} = \frac{\hbar}{mV} = \sqrt{\frac{\tilde{r}^{*2}}{2\xi^*}\frac{\hbar}{m\gamma_0}}$ – de Broglie wavelength, we easily see that in our case the rotational motion of the atom is quantum mechanical and new interesting pure quantum effects can occur.

To consider the quantum dynamics of the center-of-mass (CM) of the atomic dipole in potential (1, 6), it is necessary to solve the appropriate Schrödinger equation. Because of the spherical symmetry of the potential, a straightforward separation of variables in spherical coordinate system allows us to reduce the problem to 1D radial eigenvalue problem:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)}{r^2}\right) + U_{\mathit{eff}}(r)\right]\varphi = E\varphi. \qquad (17)$$

$$\varphi(0) = \varphi(\infty) = 0. \qquad (18)$$

Here ℓ is the orbital quantum number.

Strictly speaking, due to the singularity of potential near dielectric microsphere surface, ($U_{\mathit{eff}} \propto 1/(r-a)^3$), this problem does not have solution. So we can discuss only quasistationary states. To find the quasistationary states, one should use the boundary condition

$$\varphi(r_{min}) = \varphi(r_{max}) = 0, \qquad (19)$$

instead of equation (18), and then check the localization of wavefunctions obtained. Here, r_{min}, r_{max} are respectively the minimal and maximal values of radius characterizing the potential well.

Before solving equations (17, 19), one should note that this problem has no solution for an arbitrary atomic dipole. The point is that there are no bound states in a shallow enough well.

In the present case, the rotation of Mg atomic dipole is due to the long lifetime of the excited state, implying a small well depth, which is proportional to $\hbar\gamma_0$. Simple estimations using uncertainty principle show that there are no bound states in that case.

Indeed if we use, instead of our well, one with infinite walls at r_{min} and r_{max} , it is easy to estimate the energy of the CM ground state in the potential well:

$$E_{min} = \frac{\pi^2\hbar^2}{2m(r_{max}-r_{min})^2}\,. \qquad (20)$$

In our case $r_{min} - r_{max} \approx a/3$, so

$$\frac{E_{min}}{\hbar\gamma_0} = \frac{9\pi^2\hbar}{2ma^2\gamma_0}\,. \qquad (21)$$

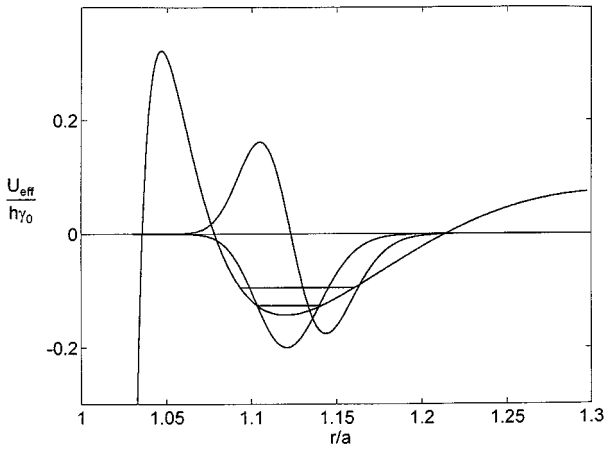


Fig. 6. Energy levels and wavefunctions for center-of-mass motion of Rb atomic oscillator ($ka = 10.488\,95$, $\epsilon = 6.01$; averaged potential; $\ell = 0$, $r_{min} = 1.03$, $r_{max} = 1.3$)

For Mg, this yields $E_{min}/\hbar\gamma_0 \approx 928$, while at the same time the total depth of our potential well, (Eq. (4)), is $E_{max}/\hbar\gamma_0 \approx 0.2$! This clearly prevents the existence of a bound quantum-mechanical state.

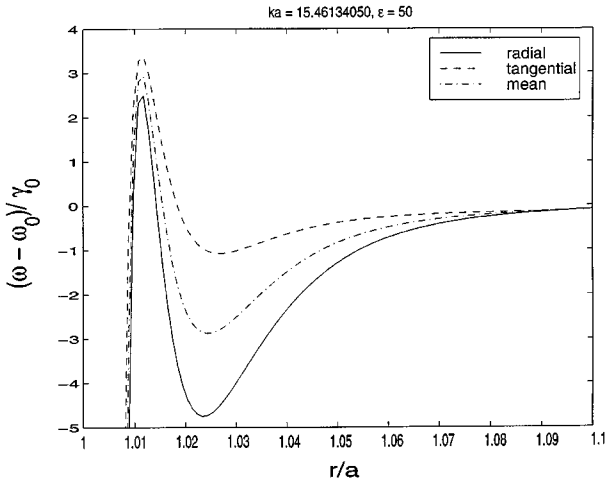
Different situations take place for the other atomic oscillators considered in Table 1. For the Rb resonance state, the energy levels and wavefunctions of the Rb center-of-mass motion (for a random orientation of the dipole momentum) are shown in Figure 6. This figure shows that CM wavefunctions with $\ell = 0$ are expected to be well-localized. So the probability for tunneling to surface should be small. States with $\ell \neq 0$ are also well-localized, because the centrifugal energy is small in comparison with the energies of low-lying levels. The same situation takes place for all atomic oscillators meeting the condition:

$$\frac{m\gamma\lambda^2}{\hbar} > 3\times 10^4. \qquad (22)$$

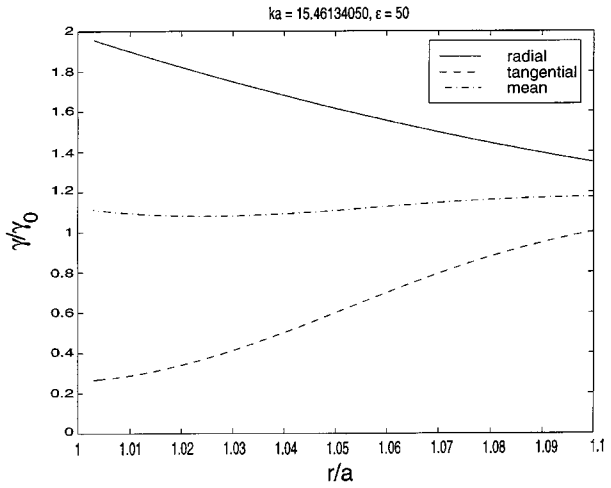
This condition ensures the existence of two well-localized states for a tangential orientation of the atomic dipole at least. Note that this orientation is less favorable for capture (see Fig. 3).

Let us now analyze the lifetime of such a system. From Figure 3b one can see that the orientation-averaged radiation line width in the case under consideration is $\gamma/\gamma_0 \approx 2$, while the potential well depth is $\Delta\omega/\gamma_0 \approx 0.2$. The comparison of these values shows that, for $\epsilon = 6$, the radiation line width exceeds substantially the potential well depth, and consequently one cannot speak of atom-microsphere exciplex, or orbital motion around the microsphere.

Nevertheless the main question remains: is it possible to predict atom's quasi orbital motion? In principle, the answer is yes if we consider a microsphere with anomalously large refraction indices. For example, for a microsphere with hypothetical index $n \approx 7$ ($\epsilon = 50$) (semiconductors in far IR range?) and with radius governed by ka =15.4613 (near the TM (1, 100, 100) Whispering Gallery Mode), the potential well depth is three times larger than the line width. The corresponding variations of



(a)



(b)

Fig. 7. Relative frequency shift $(\omega - \omega_0)/\gamma_0$ (a) and linewidth γ/γ_0 (b) as a function of the position (r/a) of the radially (solid line) and tangentially (dashed line) oscillating atomic dipole near microsphere ($ka = 15.46$ and $\epsilon = 50$). The dashed-dotted line shows the averaged frequency shift, and linewidth.

potential energy and line width for different orientations of the atomic dipole are shown in Figure 7.

A classical analysis of this potential well reveals a 5 fold increase of the revolution number for Mg (see Tab. 1, $\epsilon = 50$ column). However bound quantum levels do not arise yet for Mg.

On the other hand, with the same parameters, for *allowed* transitions, a number of well-localized energy levels exists in the potential well. The four lower levels and corresponding wave functions for Rb are shown in Figure 8.

In conclusion, we have analyzed the existence of a possible quasi orbital motion of an excited atom near a dielectric microsphere. A semi-classical analysis of this problem shows the possibility of a quasi orbital motion of an excited

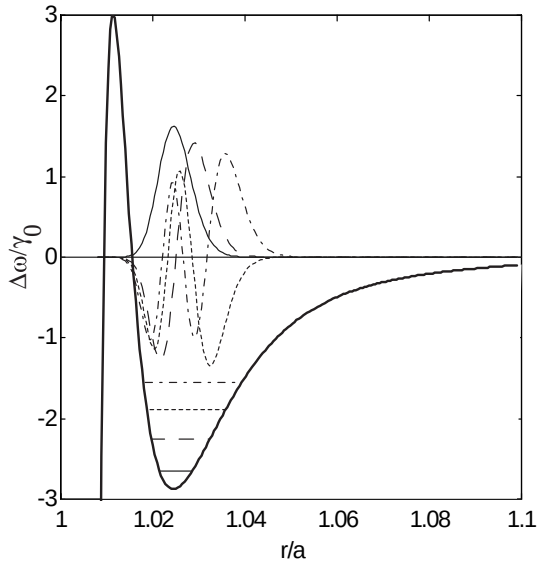


Fig. 8. Energy levels and wavefunctions for the center-of-mass motion of Rb atomic oscillator ($ka = 15.46$ and $\epsilon = 50$; averaged potential, $\ell = 0$).

atom near diamond microsphere. However, this possibility vanishes under quantum mechanical considerations.

In a quantum mechanical approach, only microspheres with a very high dielectric constant ($\epsilon = 50$) would allow for a potential well deep enough in comparison with the line width, thus making possible a quasi orbital motion for some excited atoms. In this view, the best compromise seems to be the inter combination line of Ca.

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