Calculation of the Casimir-Polder interaction between Bose-Einstein condensates and microengineered surfaces: a pairwise-summation approach

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Abstract. Understanding the Casimir-Polder (CP) attraction between ultracold atoms and dielectric surfaces is of fundamental importance to the design and miniaturization of atom chips [1] and for understanding quantum reflection from, and sticking to, the surface [2-6]. So far, calculations have focussed on planar dielectrics, either semi-infinite or of finite width [7-9], and non-planar geometries including corrugated surfaces [10], spheres and carbon nanotubes [11-12]. Here, we present a simple scheme, based on the Pairwise-Summation (PWS) approximation, for estimating the CP interaction between a ground-state alkali atom and a dielectric volume of arbitrary shape. The PWS approximation integrates the van der Waals interaction between two ground-state atoms over the many atoms in the surface volume. We relate the microscopic polarizability of atoms in the surface to the bulk dielectric constant via the Clausius-Mossotti relation within the Lorentz local-field theory. We find that the CP potential depends strongly on both the geometry and density of the surface, which modify the fluctuation spectrum of the electromagnetic field that couples the alkali atoms to the dielectric. We compare our results with known analytical expressions for the CP potential near planar surfaces and use them to investigate how BECs interact with, and may quantum reflect from, curvilinear surface structures.

1. Introduction

The ability to manipulate ultra-cold atoms using current-carrying wires microfabricated on the surface of atom chips has fuelled interest in interactions between the atoms and the chip. Understanding and reducing the intrinsic attractive interaction between an atom and a surface is crucial for trapping ultracold atoms within a micron of the surface. The reason for this is that the stability and lifetime of coherent atom clouds depend mainly on this atom-surface potential, called the Casimir-Polder (CP) potential. Classically, the CP potential can be estimated by summing the van der Waals (vdW) interaction between an atom above the surface and each atom within the surface. A full description can, however, only be explained within the framework of Quantum Electrodynamics (QED). In this approach, the CP potential results from the interaction of a single atom (in the ground or an excited state) close to a microscopic body in a quantum vacuum. The quantum vacuum fluctuations generate virtual particles that interact with the atom and the surface as predicted theoretically by Casimir and...
Polder in 1948 [13] as an extension to the vdW-London interaction between two ground-state atoms. This CP regime, also known as the vdW retarded regime, occurs when the separation between two bodies greatly exceeds the atomic transition wavelength. The CP potential of a single atom with a macroscopic body has been used to approximate the interaction between a Bose-Einstein condensate (BEC) and a surface, e.g. for quantum reflection (QR) studies [4,5]. Theoretical investigation shows that the QR probability and dynamics are both qualitatively the same for an abrupt-step potential and the exact power-law attractive CP potential [4]. Motivated by experimental studies of QR from microfabricated pillar arrays [3], here we use our PWS approximation to estimate the interaction potential between an atom and a non-planar surface, in this case a cylinder. This simple approach agrees reasonably well with exact calculations for planar surfaces and, moreover, offers the flexibility required to estimate the CP attraction to engineered surface structures of arbitrary shape.

2. Pairwise-Summation approach
We now introduce the pairwise-summation (PWS) approach to estimating the CP interaction between a single atom and a surface. There are a number of ways of understanding how this CP potential arises. The most common interpretations of the CP potential are: (i) a many-body vdW potential resulting from additive interactions between the approaching atom and each atom in the surface [12], (ii) an attraction originating from the exchange of virtual photons [8,9] between the approaching atom and the surface, and (iii) a Stark shift of the atomic energy levels [7].

The PWS approximation neglects the many-body vdW interactions between atoms within the surface. Then, the CP attraction between the approaching atom and the surface is the summation of the vdW potentials between the approaching atom and each atom in the surface, as illustrated in Figure 1. Specifically, we write the attractive CP potential in the form

\[ E_{CP} = -C_m \bar{n} \int \frac{dV}{r^m} \]

In equation (1), the interaction constant, \( C_m \), is taken from the retarded \((m = 7)\) and non-retarded \((m = 6)\) limits of the vdW atom-atom interaction [7], \( \bar{n} \) is the volume \((V)\) density of surface atoms and \( r \) is the atom-atom separation. The polarizability, \( \alpha \), of the approaching atom and the dielectric constant, \( \epsilon \), of the surface satisfy the Clausius-Mossotti (CM) relation \((\bar{n} \alpha / 3\epsilon_0) = (\epsilon - 1)/(\epsilon + 2)\) derived from Lorentz local-field theory. Comparing our PWS approach with standard expressions [1, 9] for an \(^{87}\)Rb atom approaching a planar Si dielectric, which is either semi-infinite or of finite width, we find, respectively, that equation (1) gives a 38% overestimate and a 66% underestimate of the exact results.
2.1. Non-planar surface: Cylinder

Figure 2 illustrates the interaction of an atom with a cylindrical surface. As the cylinder’s radius $R_C \to \infty$, the effect of the cylinder on the atom approaches that of a semi-infinite dielectric whose left-hand edge is shown by the bold line in Figure 2. Using equation (1), we estimate the CP potential in the retarded ($R_t$) and non-retarded ($Non-R_t$) regimes for an atom at a distance $d \leq R_C$ from an infinitely long solid dielectric cylinder as [14]

$$
E_{R_t} = -C_4 \left[ \frac{R_C^2 (R_C^2 + 2y^2)}{(y^2 - R_C^2)^4} \right] ; \quad E_{Non-R_t} = -C_3 \frac{R_C^2}{y^5} \mathcal{F} \left( \frac{5}{2} ; 2 ; \frac{R_C^2}{y^2} \right),
$$

(2)

where $y = d + R_C$, $\mathcal{F}$ is the hypergeometric function, and the interaction constants are

$$
C_4 = \frac{23\hbar c \alpha(0)}{40 \pi^2 \varepsilon_0} \left( \frac{\varepsilon - 1}{\varepsilon + 2} \right) ; \quad C_3 = \frac{27\hbar}{128 \pi \varepsilon_0} \int_0^\infty \frac{d\omega}{\omega} \alpha(i\omega) \frac{\varepsilon(i\omega) - 1}{\varepsilon(i\omega) + 2}
$$

(3)

In the limit $R_C \to \infty$ and $d \to 0$, $E_{Non-R_t}$ reduces to the CP potential for an atom near a half-plate.

Comparing CP potential values obtained from equation (2) with exact expressions (see for example Ref.[15]) for a perfectly conducting cylinder with $\varepsilon = \infty$, gives errors ranging from ~ 20% to 80% depending on the system parameters and geometry (a more detailed analysis will be presented in [16]). Here, we present PWS calculations of the retarded CP potential between a ground-state $^{87}$Rb atom near either a Si slab of finite width or a solid cylinder [Figures 3(a) and (b) respectively]. When the slab width and cylinder radius are 100 and 10 microns [top two curves in Figure 3(a,b)], these two dielectric geometries produce almost identical CP potentials when $d$ is between 1 and 10 microns. For thinner slabs and cylinders with widths or radii of 0.1 microns and 1 nm [bottom two curves in Figure 3(a,b)], the CP potential for the cylinder is significantly lower than that for the planar slab – between approximately three and four orders of magnitude lower when the slab width/cylinder radius is only 1 nm. Detailed comparison between the PWS and exact scattering approaches now needs to be done for a range of dielectric geometries and parameters in order to confirm our initial calculations.

Figure 2. Schematic interaction of an atom at distance $d$ [y] from the left-hand edge [centre] of an infinitely long cylinder (cross-section shown grey). Dashed curves show various radii of the cylinder as $R_C$ increases towards $\infty$. We calculate the CP potential by integrating the vdW potential over the surface volume: cube shows a voxel at distance $r$ from the atom.
3. Conclusion

We have used the PWS approach to calculate the CP potential for an atom near a bulk dielectric with either a planar or cylindrical geometry. We find that when the atom-surface separation is comparable to the width of a dielectric slab or the radius of a cylinder, the magnitude of the CP potential can be orders of magnitude smaller for the cylinder than for the slab. This suggests that thin or curved substrates could provide a route to trapping atoms within a micron of an atom-chip surface [4]. Although for the slab and cylinder, the PWS approach gives CP potential values that can differ by up to 100% from exact values obtained from a scattering method, it gives a fast and simple method for estimating the values and spatial variation of CP potentials for any surface geometry, e.g. MEMS devices. Our preliminary calculations show that the quantum reflection probability for a single atom approaching a surface is higher for a cylindrical dielectric than for a dielectric slab, due to the weaker CP potential of the former. We are now undertaking numerical calculations of the dynamics of Bose-Einstein condensates undergoing quantum reflection from solid and hollow cylinders with CP potentials calculated using both the PWS method and the exact scattering approach [16].

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