Interaction of atomic quantum gases with a single carbon nanotube

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received 16 January 2013; accepted in final form 25 April 2013
published online 17 May 2013

PACS 34.50.-s - Scattering of atoms and molecules
PACS 78.67.Ch - Nanotubes
PACS 67.85.-d - Ultracold gases, trapped gases

Abstract – We study inelastic processes in the hybrid quantum system constituted by a carbon nanotube (CNT) in contact with an ultracold quantum gas, such as a cloud of thermal atoms or a Bose-Einstein condensate (BEC). We present a parameter-free \textit{ab initio} approach for the loss rate based on the underlying scattering process, considering the two-dimensional character of the system as well as the exact Casimir-Polder potential. The predicted loss rates are in perfect agreement with recent experimental results, obtained both for a thermal cloud of rubidium atoms and for a BEC. For the trap loss of a thermal cloud, we find that retardation effects become important and contribute significantly, which emphasises the crucial role of the exact interaction potential.

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Introduction. – In recent years advanced techniques of cooling and controlling single atoms or ions, as well as clouds or condensates, have successfully been combined with sophisticated solid-state techniques in the production of mesoscopic structures on the nanometer scale. The emerging variety of hybrid quantum systems constitutes an interesting new field of physics [1–4]. Nanotubes, nanowires and nanorods have proven effective for constructing such hybrid systems [5–7]. These can be combined into carpets of dense standing nanotubes forming a structured surface [8,9] or to an array of nanotubes serving as a diffraction grating [10,11]. Particular attention is currently being given to the fundamental system of a single nanotube interacting with a cold gas of atoms [12–16], which lays the foundations for understanding systems of higher complexity. This is by far not a trivial problem and raises the question of the applicability of established scattering theory and nondynamical approaches [15].

In a recent experiment [12,17] Schneeweiss et al. measured the losses of atoms absorbed by a multwall carbon nanotube (length $L = 10.25\mu m$ and diameter ranging from 275 nm at the bottom to 40 nm at the tip) grown on top of a nanochip. The CNT was immersed into a BEC and in a cloud of thermal atoms and the trap loss rate $\gamma$ was measured as a function of the distance $d$ between the center of the trap and the surface of the nanochip (see fig. 1).

In this letter we present a parameter-free \textit{ab initio} description for the absorption of ultracold atoms by cylindrical geometries, based on the underlying scattering process. We show that an accurate description is possible, if the exact interaction potential is considered and the scattering process is treated properly. However, this remains nontrivial in the present case, due to the two-dimensional character of the scattering process [18–20] and due to the intricacy of the exact interaction potential [14,21]. In contrast to fitting an arbitrarily chosen model potential to the experimental data [12,17], this parameter-free approach offers a foundation for extensions to more complex hybrid systems and might assist the design of CNT-based nanodevices.

The Casimir-Polder potential. – Descriptions of an atom interacting with a cylindrical geometry go back
to Zel’dovich [22] who analyzed the interaction between an atom and a perfectly conducting cylinder in 1935. Further work on this subject extended the potential to the more realistic case of a cylinder with finite conductivity. A closed form of the full Casimir-Polder potential between an atom and a dielectric cylinder of radius \( R \) was first given by Nabutovski et al. in 1979 [23] and later by Marvin and Toigo in 1982 [24]. Though this problem has been revisited over the last years by several groups [25–27], the result obtained by Nabutovski et al. [23] is still the most general, as it covers the full Casimir-Polder potential of an atom interacting with a cylindrical geometry with arbitrary dielectric properties, including the perfectly conducting case.

The Casimir-Polder potential for a dielectric cylinder exhibits a nontrivial transition from the well-studied atom-wall potential at small atom-surface distances \((r - R)\), which is \(-C_3/(r - R)^3\), to the fully retarded asymptotic \(-C_6/r^6\) behavior far away from the cylinder. The coefficients \(C_3\) and \(C_6\) are well-defined quantities depending on both the dielectric constant of the tube and the properties of the atom, with \(C_6\) additionally depending on the radius \(R\) of the cylinder [23]. The full Casimir-Polder potential is approximated by the van der Waals potential only at very small distances and might resemble the van der Waals long-range asymptote \(-C_5/r^5\) only in a very narrow transition region. An accurate method for the numerical treatment of the full Casimir-Polder potential and, in particular, for the nontrivial transition between the van der Waals and highly retarded limit, has been developed only very recently [13,14,21].

The interaction potential between an atom and an actual CNT of finite length \(L\) obviously differs from the atom-cylinder potential [23] in a nontrivial fashion and remains in general unknown; pairwise-summation approaches [28] can in general not reproduce the correct Casimir-Polder forces [29]. Variations of the interaction energy along the tube axis are, however, small as long as the radius \(R(z)\) of the CNT varies smoothly. In this case, the longitudinal free motion of an atom along the CNT may be separated from the two-dimensional dynamics perpendicular to the tube, which is governed by the interaction potential [23] of the atom with a cylinder of radius \(R(z)\). The contribution of a single perpendicular plane to the total loss rate \(\gamma\) can be given in a differential form

\[
d\gamma(z) = n(0,0,z)K_{in}^{2D}dz,
\]

with the density of particles \(n\) around the nanotube, located at \((0,0)\) and the loss rate constant \(K_{in}^{2D}\) for inelastic and reactive scattering in this two-dimensional (2D) subsystem. These inelastic reactions (sticking, adsorption, . . .) happen at short distances to the surface and are described in the Langevin model where all atoms reaching the surface contribute to the rate constant \(K_{in}^{2D}\) [30,31]. The total trap loss \(\gamma\) of the full system is obtained by integration over all 2D planes,

\[
\gamma = \int_0^L n(0,0,z)K_{in}^{2D}dz.
\]

Deviations from this description might be expected at the tip of the nanotube where, on the one hand, the dynamics along the tube axis is influenced by the atom-cylinder potential and, on the other hand, the potential differs from the infinite cylinder potential. However, these deviations will only give small corrections to the total trap loss.

Within this description, we are able to calculate the trap loss of a Bose-Einstein condensate (BEC) and of a thermal cloud of atoms interacting with a CNT, as measured for both cases by Schneeweiss et al. [12]. All calculations presented below are based on the exact experimental parameters [17,32]. The variation of the CNT radius \(R(z)\) is assumed to be linear. The center of the cloud is shifted away from the tube in the \(z\)-direction and lies on a ray forming an angle of 13° with the \(z\)-axis [33]. Furthermore, the experimental data is, for both cases (BEC and thermal cloud), assigned to trap-surface distances measured separately with a BEC

\[\text{Absorption of a Bose-Einstein condensate. – Figure 2 shows the trap loss }\gamma\text{ for a BEC of rubidium atoms as a function of the trap-surface distance }d.\text{ The BEC is described by a macroscopic wave function in the ground state of the trap and the presence of an absorbing impurity in the cloud leads to a local depletion of its density. As a result, the condensate readjusts with the characteristic speed of sound }v_s\text{ (here 0.8 mm/s) [34] which causes a flux toward the nanotube [35]. Due to the}

\[\text{\footnotesize{The trap frequencies and temperature of the cloud slightly change with the distance [17,32].}}\]

\[\text{\footnotesize{Notice that the authors of ref. [12] relate their data for the thermal cloud to a different calibration [17], imposing a shift of 2.65 }\mu\text{m on the trap-surface distance.}}\]
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The calculated trap loss for a dielectric constant \( \varepsilon = 5 \) (solid line) reproduces the data given in [12] (full circles and error bars). The dot-dashed (dashed) line shows results for a dielectric constant \( \varepsilon = 2.5 \) \( (\varepsilon = 100) \) which leads to rather small variations in the predicted loss rates, compared to the experimental error bars.

Absorption of a thermal cloud. – The trap loss for a thermal cloud of rubidium atoms is shown in fig. 3. The velocity of the atoms in a thermal cloud is given by a Maxwell-Boltzmann distribution with \( T = 100 \) nK and the loss rate constant is given by

\[
K_{\text{in}}^{2D} = 2\pi v_{\perp}\sigma_{\text{abs}}(m=0)(v_{\perp}),
\]

(3)

The density of the BEC in a harmonic trap is given by a Thomas-Fermi distribution [34], with the characteristic Thomas-Fermi radii, \( r_{x}^{\text{TF}} = 16 \) \( \mu \)m, \( r_{y}^{\text{TF}} = r_{z}^{\text{TF}} = 3.2 \) \( \mu \)m. As the number of atoms in the condensate decreases during the absorption process, the Thomas-Fermi radii and the speed of sound do not stay constant over time, which leads to an algebraic instead of an exponential decay [35]. These corrections and possible fluctuations due to collective oscillations [12,15] lie within the experimental error bars. The influence of the nanochip on the trap loss can be neglected for distances \( d \) larger than \( 5 \) \( \mu \)m [12]. The cross section \( \sigma_{\text{abs}}^{(m=0)} \) is calculated using well-established scattering theory [18,31] and the full Casimir-Polder potential [23] as well as incoming boundary conditions for the description of inelastic collisions at the surface of the nanotube [14,36,37].

The Casimir-Polder potential depends generally on the nontrivial dielectric properties \( \varepsilon(\omega) \) of a multilayer film [20–42]. For the actual nanotube used in the experimental setup of Schneeweiß et al. [12] these are not known. In our ansatz we use a frequency-independent dielectric constant \( \varepsilon \) in the range from \( \varepsilon = 2.5 \) (dotted-dashed line) up to \( \varepsilon = 100 \) (dashed line), which reproduces the experimental data shown in fig. 2 (full circles). Variations of \( \varepsilon \) in this wide range have — compared to the experimental error bars — only a small impact on the theoretical prediction for the trap loss. A detailed knowledge of the dielectric properties is thus not essential for the description of the experimental results of ref. [12].

For the case of a thermal cloud we also performed a time-dependent three-dimensional classical simulation

![Fig. 2](image-url) (Color online) Trap loss \( \gamma \) for a BEC of rubidium atoms overlapping with a carbon nanotube. The calculated trap loss for a dielectric constant \( \varepsilon = 5 \) (solid line) reproduces the data given in [12] (full circles and error bars). The dot-dashed (dashed) line shows results for a dielectric constant \( \varepsilon = 2.5 \) \( (\varepsilon = 100) \) which leads to rather small variations in the predicted loss rates, compared to the experimental error bars.

![Fig. 3](image-url) (Color online) Trap loss \( \gamma \) for a thermal cloud of rubidium atoms overlapping with a carbon nanotube. The black solid line shows the predicted trap loss for a dielectric constant \( \varepsilon = 5 \) which is in good agreement with the experimental results [12] (full circles and error bars). The blue triangles show a three-dimensional classical simulation of the system which reproduces the predicted classical trap loss (blue dashed line) and shows rather small deviations from the quantum-mechanical results.
The results obtained with the full Casimir-Polder potential from curves in fig. 5), within a wide range of dielectric constants. The van der Waals potential fails to describe the trap loss (upper curves) and on the van der Waals potential only, where retardation effects are neglected (upper curves). The shaded area shows loss rates for dielectric constant of the nanotube in a regime from $\varepsilon = 2.5$ (dot-dashed line) up to $\varepsilon = 100$ (dashed line). The solid line shows the trap loss for a dielectric constant of $\varepsilon = 5$. The experimental data [12] (full circles) clearly deviates from the prediction calculated with the van der Waals potential only.

**Conclusion.** – In this letter, an accurate parameter-free ab initio description of the trap loss in a hybrid system consisting of a single nanotube immersed in an ultracold atomic quantum gas, such as a thermal cloud or a BEC, is presented. A quantum-mechanical calculation of the absorption cross section based on the exact Casimir-Polder potential leads to perfect agreement with recent experiments [12], both for a thermal cloud and for a BEC. Furthermore, it has been shown that the van der Waals potential fails to reproduce the loss rates of a thermal cloud of atoms; retardation effects that are accounted for in the Casimir-Polder potential need to be considered. An accurate description of this hybrid system is achieved with a proper use of scattering theory together with the exact Casimir-Polder potential. The present approach gives insight into the underlying processes and therefore promotes a deeper understanding of hybrid systems, which is essential for the design of future nanodevices.

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The authors thank J. FORTÁGH, A. GÜNTER, P. SCHNEEWIESS, T. E. JUDD for providing experimental parameters and for helpful discussions. Useful input by
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