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Atomic Spin Flip Loss and Spatial Decoherence

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Abstract. We present a first-principles derivation of spatial atomic-sublevel decoherence near dielectric and metallic surfaces. We find that for small lateral separations of the atom's possible positions, the spatial decoherence decreases quadratically with the separation and inversely to the squared atom–surface distance. In view of potential miniaturization of atom optics, we also present preliminary results on spin flips times near a metallic carbon nanotube.

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1. Introduction

New physical models for quantum information processing and quantum computation have been inspired by the recent experimental achievements in controlling ultracold neutral atoms [1–5]. The creation of microscopic traps and guides for neutral atoms moving close to surfaces is possible using nanofabricated structures. The principal idea of how to design magnetic traps can be traced back to Frisch and Segré [6] who realized that, when a homogeneous magnetic field is superimposed with the field created by a current flowing through a wire, the magnetic field vanishes on a line parallel to the current. Such a configuration is used to trap atoms in low-field seeking magnetic hyperfine sublevels. One of the challenges in trapping ultracold atoms is now to reduce as much as possible the dimension of the atomic traps. It is well known that carbon nanotubes (CNs) have attractive mechanical and electrical properties for applications in electronic devices. Due to these promising properties, CNs used as current carrying wires may be regarded as promising candidates in the miniaturization of atomic traps.

However, atoms kept in traps are held close to microstructured material surfaces, which are typically at room temperature. The small separation between the cold atom cloud and the macroscopic environment raises the question of how strong

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the energy exchange will be, and which minimal distance from the surface can be ultimately reached. In the materials generating the trapping electromagnetic field, dissipation processes associated with finite conductivity give rise to electromagnetic field fluctuations. Such fluctuating fields can be strong enough for an atom close to the surface to drive rf magnetic dipole transitions that flip its spin causing either its loss from the trap or decoherence of its quantum state. In [4, 7–12], atom loss due to thermally driven spin flips has been investigated and several experiments have confirmed the theoretical findings [13–15]. In this article we examine the influence of thermally-induced spin flips on the lifetime of an atom trapped near a CN and on the coherence properties of atomic spatial superposition states. Such coherent superpositions can be thought of being created by tunnelling through a shallow potential barrier in either a double-well potential or, more generally, an optical lattice structure [16–18].

This work is organized as follows: Sec. 2 introduces the basic notions of QED in dielectric media. In Sec. 3 an expression for the spatial coherence is derived. We focus on a planarly multilayered structured in Sec. 4, for which the dyadic Green function is explicitly known and finally, in Sec. 5 we introduce our preliminary results for CNs.

2. Basic Equations

In the present context it is useful to formulate quantum electrodynamics (QED) on a dielectric-matter background [19]. Let us restrict our attention to an isotropic but arbitrarily inhomogeneous medium whose polarization responds linearly and locally to the electric field. Causality and the dissipation-fluctuation theorem [20] then require the macroscopic polarization $\hat{\mathbf{P}}(\mathbf{r},t)$ to be a convolution of the dielectric susceptibility $\chi(\mathbf{r},t)$ and the electric field $\hat{\mathbf{E}}(\mathbf{r},t)$ plus a noise polarization $\hat{\mathbf{P}}_N(\mathbf{r},t)$ that accounts for the quantum fluctuations of the macroscopic polarization. Using Maxwell's equations in Fourier space, and solving the Helmholtz equation for $\hat{\mathbf{E}}(\mathbf{r},\omega)$, we get

$$\hat{\mathbf{E}}(\mathbf{r},\omega) = \omega^2\mu_0 \int d^3\mathbf{r}' \boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega)\cdot\hat{\mathbf{P}}_N(\mathbf{r}',\omega)\,, \tag{1}$$

where the Green tensor $\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega)$ is a second rank tensor determined from the partial differential equation

$$\nabla\times\nabla\times\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega) - \frac{\omega^2}{c^2}\varepsilon(\mathbf{r},\omega)\,\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r}-\mathbf{r}')\,\boldsymbol{U}\,, \tag{2}$$

with $\varepsilon(\mathbf{r},\omega)$ the complex permittivity. Together with the boundary condition at infinity, this equation has an unique solution. The corresponding solution for the magnetic field in Fourier space is $\hat{\mathbf{B}}(\mathbf{r},\omega) = (i\omega)^{-1}\nabla\times\hat{\mathbf{E}}(\mathbf{r},\omega)$.

The noise polarization is given by

$$\hat{\mathbf{P}}_N(\mathbf{r},\omega) = i\sqrt{\frac{\hbar\varepsilon_0}{\pi}\varepsilon_I(\mathbf{r},\omega)}\,\hat{\mathbf{f}}(\mathbf{r},\omega)\,. \tag{3}$$

where the operator-valued bosonic vector field $\hat{\mathbf{f}}(\mathbf{r},\omega)$ represents the collective excitation of the combined system of the electromagnetic field and absorbing matter and satisfies the equal-time commutation relations $[\hat{\mathbf{f}}(\mathbf{r},\omega),\hat{\mathbf{f}}^\dagger(\mathbf{r}',\omega')] = \delta(\mathbf{r}-\mathbf{r}')\times \delta(\omega-\omega')\,\boldsymbol{U}$. The Hamiltonian of the medium-assisted electromagnetic field can be written as

$$\hat{H}_F = \int d^3\mathbf{r} \int_0^\infty d\omega\, \hbar\omega\, \hat{\mathbf{f}}^\dagger(\mathbf{r},\omega)\cdot\hat{\mathbf{f}}(\mathbf{r},\omega)\,. \tag{4}$$

Such a quantization model provides a valid description of the quantized electromagnetic field in absorbing dielectric materials. However, it is necessary to point out that a strictly local response has been assumed which neglects effects stemming from motion of charge carriers.

For the purpose of the present paper we need to calculate certain field correlation functions. Let the system of electromagnetic field and absorbing matter be in thermal equilibrium at some temperature T. Then the thermal correlation function of the magnetic induction at temperature T reads

$$\langle\hat{\mathbf{B}}(\mathbf{r},\omega)\hat{\mathbf{B}}^\dagger(\mathbf{r}',\omega')\rangle = \frac{\hbar\mu_0}{\pi}\mathrm{Im}\left[\overrightarrow{\boldsymbol{\nabla}}\times\boldsymbol{G}(\mathbf{r},\mathbf{r}',\omega)\times\overleftarrow{\boldsymbol{\nabla}}\right](\bar{n}_{\mathrm{th}}+1)\,\delta(\omega-\omega')\,. \tag{5}$$

with $\bar{n}_{\mathrm{th}}$ the mean thermal photon number at a given frequency ω. It is worth noting that this correlation function gives information about the coherence properties of the magnetic field fluctuation produced by the medium considered.

3. Spin Flip Rate and Spatial Decoherence

An atom in a magnetic trap is subject to a constant magnetic field with strength B_0 in the centre of the trap. The magnetic sublevels are split due to the Zeeman effect. In the experiment reported in [13] ^{87}Rb atoms are initially pumped into the hyperfine state $|F,m_F\rangle = |2,2\rangle$ in which they are trapped. However, due to absorption in the surface material and the resulting quantum fluctuations, fluctuating magnetic fields cause the atoms to evolve into states with lower magnetic quantum number m_F. In sufficiently tight magnetic traps, atoms in the $|F,m_F\rangle = |2,1\rangle$ state are also trapped. Spin flips to even lower magnetic sublevels cause the atoms to be expelled from the trap.

The Zeeman coupling of the atomic magnetic moment to a fluctuating field is represented by the Hamiltonian $\hat{H}_Z = -\hat{\boldsymbol{\mu}}\cdot\hat{\mathbf{B}}(\mathbf{r}_A)$, where the magnetic moment vector is associated with a transition $|i\rangle \to |f\rangle$ from the initial to the final state, as explained in [10,21]. Its modulus is proportional to the expectation value of the electronic spin operator $\boldsymbol{\mu} = g_S\mu_B\langle i|\hat{\mathbf{S}}|f\rangle$, where μ_B denotes the Bohr magneton, and $g_S \approx 2$ the electron's g-factor. The Zeeman Hamiltonian can be written in the rotating-wave approximation as [10]

$$\hat{H}_Z = -\mu_B g_S\left[\langle f|\hat{S}_q|i\rangle\hat{\xi}^\dagger\hat{B}_q(\mathbf{r}_A) + \mathrm{h.c.}\right], \tag{6}$$

where $\hat{\xi} = |f\rangle\langle i|$ denotes the atomic spin lowering operator. Finally, the free atomic Hamiltonian can be written in the two-level approximation used above as $\hat{H}_A = \hbar\omega_A\hat{\xi}_z$, where the $\hat{\xi}$ obey the commutation rules $[\hat{\xi}^{(\dagger)}, \hat{\xi}_z] = \mp\hat{\xi}^{(\dagger)}$.

Let us consider a system composed of the two-level atom and a fluctuating magnetic field initially in the vacuum state $|0\rangle$. The Hamiltonian describing the evolution of the combined system is given by the sum of the three Hamiltonians $\hat{H} = \hat{H}_F + \hat{H}_A + \hat{H}_Z$. To study spatial decoherence in this context, we consider an atom in a superposition of two different sites and we are going to look at the off-diagonal term of its density matrix. We can write the system wave function at a certain time t as [22]

$$\begin{aligned}|\psi_{AF}(t)\rangle &= C_{i_1}(t)e^{-i\omega_A t/2}|i_1,0\rangle + C_{i_2}(t)e^{-i\omega_A t/2}|i_2,0\rangle \\ &+ \int d^3\mathbf{r}\int_0^\infty d\omega\, C_{f_1,m}(\mathbf{r},\omega,t)e^{-i(\omega-\omega_A/2)t}|f_1,1_m(\mathbf{r},\omega)\rangle \\ &+ \int d^3\mathbf{r}\int_0^\infty d\omega\, C_{f_2,m}(\mathbf{r},\omega,t)e^{-i(\omega-\omega_A/2)t}|f_2,1_m(\mathbf{r},\omega)\rangle\,, \end{aligned} \tag{7}$$

where $|0\rangle$ and $|1_m(\mathbf{r},\omega)\rangle$ denote the electromagnetic field vacuum and single-excitation states, respectively, and the labels $1,2$ refer to the occupied site. After solving the Schrödinger equation $i\hbar\partial_t|\psi_{AF}(t)\rangle = \hat{H}|\psi_{AF}(t)\rangle$ as explained in [21] and defining the coefficients

$$\Gamma_a = 2\left(\frac{(\mu_B g_S)^2}{c^2\varepsilon_0\hbar}\right)\langle f|\hat{S}_q|i\rangle\langle i|\hat{S}_k|f\rangle \mathrm{Im}\left[\overrightarrow{\boldsymbol{\nabla}}\times\boldsymbol{G}(\mathbf{r}_a,\mathbf{r}_a,\omega_A)\times\overleftarrow{\boldsymbol{\nabla}}\right]_{qk} \tag{8}$$

and

$$\delta\omega_a = \left(\frac{(\mu_B g_S)^2}{c^2\pi\varepsilon_0\hbar}\right)\langle f|\hat{S}_q|i\rangle\langle i|\hat{S}_k|f\rangle\mathcal{P}\int_0^\infty d\omega\frac{\mathrm{Im}\left[\overrightarrow{\boldsymbol{\nabla}}\times\boldsymbol{G}(\mathbf{r}_a,\mathbf{r}_a,\omega)\times\overleftarrow{\boldsymbol{\nabla}}\right]_{qk}}{\omega-\omega_A}\,, \tag{9}$$

we can write the time evolution of the coefficients $C_{i_a}(t)$ as

$$C_{i_a}(t) = \exp\left[\left(-\frac{1}{2}\Gamma_a + i\delta\omega_a\right)t\right]. \tag{10}$$

The coefficients Γ_a and $\delta\omega_a$ defined in Eqs. (8) and (9) represent the spin flip rate and the line shift, respectively, and have been derived in a similar fashion in [10]. In order to investigate spatial decoherence we want to analyse the decay of the off-diagonal elements of the density matrix of our system written in the occupation-number basis. After tracing the system density matrix over the field, the off-diagonal element of the atomic density matrix is given by

$$\varrho_{12}(t) = e^{-\Gamma_{12}t} + 2\left(1 - e^{-\Gamma_{12}t}\right) \frac{(\mu_B g_S)^2}{c^2 \varepsilon_0 \hbar} \langle i|\hat{S}_q|f\rangle\langle f|\hat{S}_k|i\rangle \times \frac{\mathrm{Im}\left[\overrightarrow{\nabla} \times \boldsymbol{G}(\mathbf{r}_2, \mathbf{r}_1, \omega_A) \times \overleftarrow{\nabla}\right]_{kq}}{\Gamma_{12}}, \tag{11}$$

where $\Gamma_{12} = (\Gamma_1 + \Gamma_2)/2$ is the arithmetic mean of the spin flip rates, Eq. (8), at both sites. Equation (11) consists of two parts. The first is a (spatially local) exponential decay that describes the effect of the transition from the initial spin state $|i\rangle$ to the final spin state $|f\rangle$. The second term is a (spatially nonlocal) non-exponential term which is proportional to the spatial coherence function of the magnetic induction defined in Eq. (5). It means that by observing the spatial decoherence of our system we gain information about the magnetic-field fluctuations produced by the substrate.

4. Planar Substrates

Up until now, the derivation of all formulas were valid for arbitrary substrate geometries. A particular geometric arrangement is fixed by defining the correct boundary conditions for the dyadic Green function $\boldsymbol{G}(\mathbf{r}, \mathbf{s}, \omega)$. In this section, we will concentrate on the simplest but experimentally important realization in terms of planar multilayer dielectrics focusing on the spatially nonlocal term in Eq. (11) only. In particular, we notice that this is equivalent to taking the long-time limit of Eq. (11). Hence, for now we consider only

$$S(\mathbf{r}_1, \mathbf{r}_2, \omega_A) = 2\frac{(\mu_B g_S)^2}{c^2 \varepsilon_0 \hbar} \langle i|\hat{S}_q|f\rangle\langle f|\hat{S}_k|i\rangle \frac{\mathrm{Im}\left[\overrightarrow{\nabla} \times \boldsymbol{G}(\mathbf{r}_2, \mathbf{r}_1, \omega_A) \times \overleftarrow{\nabla}\right]_{kq}}{\Gamma_{12}}. \tag{12}$$

The dyadic Green function for this situation can be found in [21, 23, 24]. Let us assume that an atom is located at a distance d away from a planar interface with a metallic substrate which we describe by its skin depth δ. In our example, we have chosen an aluminium substrate with $\delta = 110$ μm and an atomic transition frequency of $f = 560$ kHz. Furthermore, the atom can be in two distinct positions with a lateral separation l.

In Fig. 1 we show the decay of the spatial coherence as measured by the function $S(\mathbf{r}_1, \mathbf{r}_2, \omega_A)$ for varying separation l in μm for three different atom–surface distances d. As a function of separation, the decay of the spatial coherence starts off rather slowly. We attribute this behaviour to the fact that for separations below the coherence length of the magnetic-field fluctuations the spin flip is driven coherently at both sites.

In order to investigate the small-separation limit in some more detail, we take a closer look at the expansion of the scattering Green tensor and in certain asymptotic regimes in which Γ_{12} can be expressed as a monomial $\propto d^{-n}$ of the atom–surface

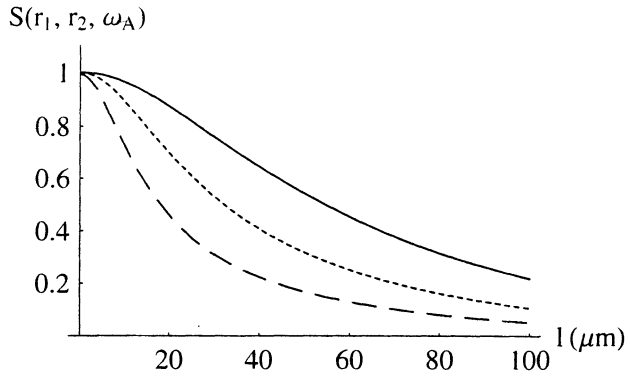

Fig. 1. Spatial coherence function of the fluctuating magnetic field $S(\mathbf{r}_1, \mathbf{r}_2, \omega_A)$, Eq. (12), as a function of the lateral separation l in μm with the parameters $f = 560$ kHz, $\delta = 110$ μm for three different distances from the surface: $d = 20$ μm (solid line), $d = 10$ μm (dotted line), and $d = 5$ μm (dashed line)

distance d (see, e.g. [8,12]), Eq. (12) can be rewritten in the form

$$S(\mathbf{r}_1, \mathbf{r}_2, \omega_A) = 1 - \frac{5n(n+1)l^2}{96d^2} + \mathcal{O}(l^4)\,. \tag{13}$$

In addition to the planar half-space we consider the experimentally relevant situation in which a thin metallic layer of thickness h has been brought onto a dielectric substrate. In order to see how the time scale is related to the expected lifetime we can expand the exponential in Eq. (11) for short times as [21] and substitute Eq. (13) obtaining

$$|\varrho_{12}(t) - \varrho_{12}(0)| \cong \frac{5\alpha l^2}{48d^2}\left(\frac{t}{\tau}\right) + \mathcal{O}(t^2)\,, \tag{14}$$

where $\varrho_{12}(0) = 1$ and $\tau = \Gamma_{12}^{-1}$ and with $\alpha = 1$ for thick films and $\alpha = 3$ for thin films. The left-hand side in Eq. (14) can be thought as a proper measure of decoherence due to spin flips in terms of physical parameters such as the spin flip lifetime τ, the separation l and the distance from the surface d. This means that it is possible to maximize those experimental parameters while the decoherence rate is under control. Hence, Eq. (14) turns out to be particularly interesting from the quantum information point of view when a certain degree of spatial coherence has to be maintained.

5. Spin Flips near Carbon Nanotubes

One of the aims of atom optics is to miniaturize its devices to even smaller scales. It is well known that CNs are useful in the miniaturization of many different devices

such as electronic, mechanical, electromechanical, chemical and scanning probe devices. A metallic CN may be considered as an infinitely thin conducting cylinder. Ideally, one can think of miniaturizing atom chips by using a metallic CN as a conducting wire to trap an atom.

In order to describe the interaction of an atom with the CN, we adopt the theory of QED in dielectrics as before for bulk materials, [25]. The use of this theory is correct if a CN may be considered as a mesoscopic object. CNs are probably at the limit to what we can actually describe with this macroscopic theory. If an atom is placed far enough from the surface, say a few nanometers, the CN is seen as an homogeneous object by the probe atom so that the detailed structure from the surface cannot be resolved and QED in dielectrics safely can be used.

It is interesting to look at the actual lifetime of an atom trapped close to a CN in the same fashion as in [10]. The Green function with the appropriate boundary conditions at the surface and the conductivity are given in [25, 26]. We evaluate Eq. (8) for three different distances d from the surface of a metallic CN: $d_1 = 1$ nm, $d_2 = 10$ nm and $d_3 = 100$ nm and we obtain for the respective lifetimes (at room temperature) the following results $\tau_1 = 0.089$ s, $\tau_2 = 2.623$ s and $\tau_3 = 178.8$ s [27]. From these preliminary values, the trapping of atoms a few nm away from a CN seems feasible when taking into consideration thermal spin flips.

6. Conclusions

In summary, we have investigated the loss of spatial coherence of atomic superpositions due to thermally driven spin flips. The consistent quantization of the electromagnetic field in absorbing dielectrics and metals allowed us to employ a first-principles approach to decoherence in this particularly simple physical system. For small lateral separation l of the atom's two possible positions we found that the spatial coherence decreases quadratically with l and inversely proportional to the squared atom–surface distance d [Eq. (13)].

We believe that these results are important for the design of microstructured devices in which spatial coherences are used to encode quantum information. In particular Eq. (14) shows how the decoherence rate depends on experimental parameters such as lifetime, lateral separation and atom–surface distance.

Finally, our estimations for CNs seem to suggest that the trapping of atoms a few nanometers away from a CN surface is achievable.

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