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Magnetically induced anions

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Abstract. We study non-conventional states of singly negatively charged ions which are supported exclusively due to the presence of an external magnetic field and have no counterparts in the field-free space. Such states experience a significant impact due to the motional effects of an anion as an entity across the magnetic field. We briefly outline the physical insight and the state-of-the-art concerning the magnetically bound anions.

1. Introduction

The behavior and properties of negative ions have been the subject of intense research for many decades. There exists a vivid interest in the electronic structure and dynamics of negative ions, both from the theoretical and experimental points of view (see, e.g., [1, 2], and the references therein). The formation and binding mechanisms of negative ions are of delicate nature. Most neutral atomic and small molecular species lead to anions with a few bound states. In some cases even no anionic counterpart exists. Therefore there is a lot of special interest to anions in external fields that add significantly to the variety of anionic states as well as to the richness of their properties. Focusing on magnetic fields a key work was done by Avron, Herbst and Simon [3] who arrived at the surprising statement that any anion possesses an infinite number of bound states for arbitrary magnetic field strength. Motivated by this spectacular discovery a number of investigations on the physical properties of these newly formed anions have been recently performed. Particular attention has been paid to developing a theoretical approach which goes beyond the assumption of an infinitely heavy nucleus that was applied in [3]. The latter assumption has been found to be too crude when treating the magnetically bound anions. Including effects due to the collective motion of such anions has been shown to possess a severe impact on their spectral and dynamical properties. In the following sections we first discuss the physics of an infinite manifold of the magnetically bound anions within the approximation of the infinitely heavy (i.e. fixed in space) nuclei. Afterwards we describe the role of the motional effects due to the finite mass of the anions. In particular we draw attention to classical simulations which show that the motion-induced dynamics can lead to a decay of the magnetically induced states. Brief conclusions and outlook to further relevant investigations on magnetically bound anions are given at the end.

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2. Static anions: infinite manifold of magnetically induced bound states

The assumption that the anion is static (infinitely heavy) reduces the problem of its binding to the investigation of the electronic motion only. Such an approach has been exploited in [3] to come to the conclusion that there are infinitely many bound states of any anion in the presence of an external magnetic field. However the corresponding consideration was a very formal and purely mathematical one employing advanced techniques from functional analysis. In [4] several transparent physical approximations have been applied and justified in the course of the estimation of the binding energies of the magnetically supported anionic states. The basic features of the underlying picture can be summarized as follows:

- A neutral atom or a small molecule plays a role of a *static attractive center* exerting on the extra electron a potential $V(\mathbf{r})$. For the species which do not possess a permanent dipole moment this potential is a polarization-like one at large distances r of the extra electron from the neutral system.
- The external electron is *additionally confined in two dimensions*, in the plane transverse to the magnetic field.
- The component of the angular momentum of the excess electron along the field is an *integral of motion*.

Within such a picture, binding of an extra electron by a neutral species can be treated as a *one-dimensional problem*, for the motion of the electronic guiding center along the magnetic field. The electron can be attached with different longitudinal angular momenta, $l_z = -s$, where $s = 0, 1, 2, \dots$, and for each s a different potential emerges. The corresponding loosely bound states constitute an infinite manifold, and their binding energies are

$$\varepsilon_0 = 0.31\kappa^2 B^2, \quad s = 0, \quad (1)$$

$$\varepsilon_s = 0.12\kappa^2 B^3 \delta_s^2, \quad s = 1, 2, \dots, \quad (2)$$

$$\delta_1 = 1, \quad \delta_s = [1 - (1.5/s)]\delta_{s-1},$$

where κ is the scalar polarizability of the neutral species and B is the magnetic field strength, both in atomic units. It is important to note that the magnetically induced states with $s > 0$ are supported exclusively by the long-range polarization attraction of the electron to the neutral species. For the magnetically bound $s = 0$ state, the short-range behavior of the potential $V(\mathbf{r})$ is relevant. This state also typically possesses the same symmetries as the conventional anionic state in case the latter exists. Therefore the $s = 0$ state can only manifest itself for the species which do not form stable anions in the absence of the magnetic field.

3. Beyond the approximation of spatially fixed (static) anions

When one takes into account that the anion can move as an entity, the formation of magnetically induced states differs in a number of important aspects from the case of a fixed nucleus:

- The external electron is still attracted by the neutral species owing to a polarization-like potential, but the latter potential is *no longer exerted by a static center*.
- The transverse motion of the external electron is still confined, by the magnetic field, in a laboratory reference system. It is, however, *no longer confined with respect to the location of the neutral species* since the latter can move.
- The electronic longitudinal angular momentum is *no longer an integral of motion*.

Within a relevant approach, binding of an extra electron becomes now a *three-dimensional problem*. The corresponding degrees of freedom relate to the motion of the guiding center of the excess electron along the magnetic field and to the motion of the neutral species across the field. These degrees of

freedom are inherently coupled to each other, and the coupling can make the magnetically induced states *autodetaching* [5].

For the details we address the reader to [6] where a rigorous theoretical approach has been developed resulting in a description of the dynamics of the magnetically induced anionic states in terms of the coupled degrees of freedom mentioned above. A meaningful Hamiltonian has been derived that involves as an essential ingredient a two-dimensional potential, $V_{\text{eff}} = V_{\text{eff}}(z, r_c)$, depending on the longitudinal, z , and the transverse, r_c , displacements of the guiding center of the extra electron from the neutral anionic counterpart. The latter potential is a prevailing potential which links the loosely bound excess electron to the moving neutral species. It should be noted that although the derived Hamiltonian has a reasonably low dimensionality, in the framework of a quantum description the potential involved depends on a canonical pair of coordinate and momentum and is non-local. This complicates investigation of its properties by direct quantum methods. In [7] this Hamiltonian has been applied to study the classical dynamics of moving magnetically induced anions. The classical simulations have been carried out for the initial conditions corresponding to the bound anion in the absence of the coupling between the motions of the neutral species and the extra electron. Starting from such conditions, the classical trajectories have been propagated taking into account the motional coupling and thereby elucidating its role for the dynamics of the anion. An initially stable anion was assumed to perform, as a single charge, a Larmor rotation in the plane transverse to the magnetic field, with the extra electron bound to the neutral species such as for a static anion. The corresponding energy shells were defined by two quantum numbers,

$$E_{Ns} = \frac{B}{M} \left(N + \frac{1}{2} \right) - \frac{\mu}{m_e} \varepsilon_s, \quad N = 0, 1, 2, \dots, \quad s = 0, 1, 2, \dots, \quad (3)$$

where $M = m_{\text{at}} + m_e$ is the total mass of the anion, $\mu = m_e m_{\text{at}} / M$ is the reduced mass of the excess electron (m_e and m_{at} are the electronic mass and the mass of the neutral species, respectively) while ε_s is the binding energy of the extra electron in a static anion.

Figure 1 shows the atomic trajectories for a positive value of the energy shell from equation (3) which corresponds to an initial excitation of the anion Cs^- according to $N = 10$, $s = 1$ in a magnetic field $B = 10$ T. The propagated trajectories relate to the different integer values of an integral of motion, \mathcal{L} , which is the total longitudinal angular momentum of the extra electron and the neutral atom. We found that smaller values of \mathcal{L} correspond to a more efficient fluctuating energy exchange between the atomic and the electronic degrees of freedom which trigger the autodetachment process. For larger \mathcal{L} these fluctuations are insufficient to cause the autodetachment. When the anion undergoes detachment, the atomic motion becomes unbound, finally resulting in a straight trajectory. For a bound anion the atom follows circular-like orbits. In figure 2, the electronic motion corresponding to two atomic trajectories, a detaching one and a bound one, is presented. For the detaching motion both the longitudinal (z) and transverse (r_c) separation between the atom and the electronic guiding center increase unlimited with time. For the bound anion, both displacements oscillate with time, and the amplitude as well as the frequency of the fast oscillations of z are modulated by the slower oscillations of r_c .

Figures 3 and 4 demonstrate the results of statistical studies of the decay of the initially bound anionic states via the motion-induced coupling. Classical trajectories have been propagated corresponding to different initial conditions associated with a certain energy shell (3). For each trajectory of such an ensemble the detachment time has been calculated, being a measure of the time required to change the character of motion from initially bound to an unbound one. In this way autodetachment curves have been obtained which show the fraction of detached trajectories depending on the propagation time. As a relevant example figure 3 shows the detachment curve for the ion H^- moving in a typical laboratory magnetic field $B = 1$ T. The lowest energy shell of equation (3) for $N = s = 0$ has been selected, which is positive, $E_{Ns} = 1.046 \times 10^{-9}$ a.u., and therefore relates to autodetachment. The classical simulations show that the autodetachment process is essentially completed for the complete ensemble of trajectories within 12 ns. This time scale is a measure for the lifetime of the anion H^- prepared initially in the $N = s = 0$ state. Also shown in figure 3 are the typical detaching trajectories associated with the different

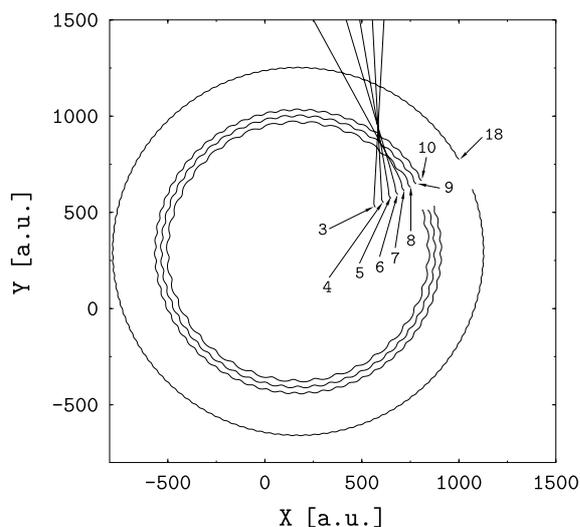


Figure 1. Atomic trajectories for the motion of a Cs^- ion across the magnetic field $B = 10$ T. The different trajectories relate to the different values of the total longitudinal angular momentum \mathcal{L} indicated at the arrows which point to the initial locations of the atom.

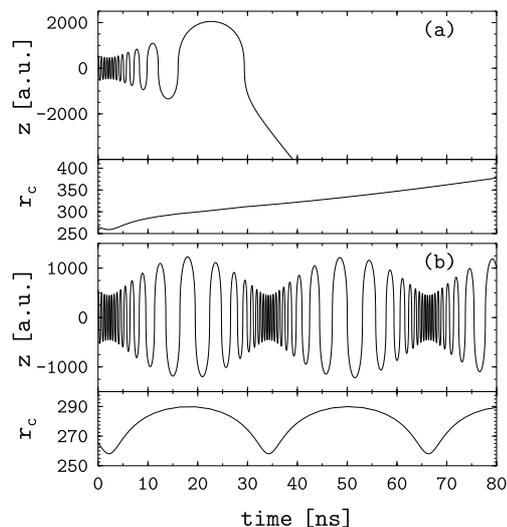


Figure 2. The motion of the extra electron for selected atomic trajectories of the anion Cs^- . Subfigures (a) and (b) correspond to values of the total longitudinal angular momentum of $\mathcal{L} = 7$ and 8 , respectively.

parts of the autodetachment curve. Figure 4 illustrates the autodetachment decay of the magnetically induced Cs^- anion. This anion is much heavier than H^- and therefore expected to be more stable with respect to the motion-induced coupling. Besides, for fixed a nucleus, its magnetically induced states are more strongly bound, due to the large polarizability of the Cs atom. For the same magnetic field strength, $B = 1$ T, the energy shell (3) for the anion Cs^- corresponding to $N = s = 0$ is negative, providing a stable bound motion. For $N = 0$ and higher s the energy shells are positive. The corresponding states undergo the autodetachment process, and the related curves demonstrate the interesting feature that for higher internal excitations of the anion its motion-induced decay is much slower than for low excitations. For example, the typical time for the complete autodetachment decay of all anionic configurations $N = 0$, $s = 2$ is 3000 ns, which is by a factor of two larger than the corresponding time of 1400 ns for the decay of the anions initially prepared for $N = 0$, $s = 1$. Extrapolating this classical feature to properties of quantum states of the magnetically induced anions one may expect that the energetically higher resonance states have longer lifetimes.

4. Conclusions and Outlook

Magnetically induced anions are challenging examples of quantum systems where the effects due to the collective motion play an essential role in the determination of the physical properties of the species. The corresponding states are also of major interest to be detected experimentally, especially for those anions which *do not exist in the absence of the field* (like, e.g., Ar^- and Xe^-). Further necessary theoretical efforts will focus on the treatment of the coupling between the motions of the neutral species and the external electron in the magnetic field in the framework of a quantum approach. Some relevant possibilities to proceed have recently been suggested in [8] and the corresponding theoretical investigations are now in progress. They are expected to provide new fundamental knowledge on a rich spectrum of bound and resonance states of the anions moving in magnetic fields.

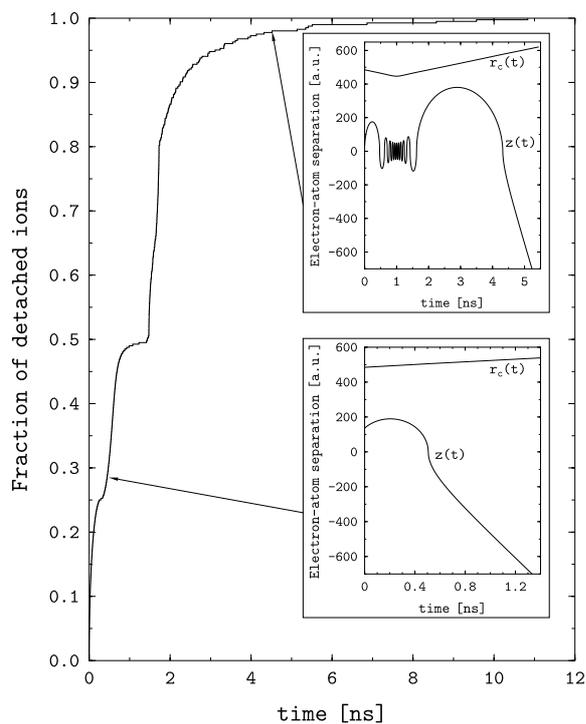


Figure 3. The fraction of trajectories which describe the detachment of the extra electron from the anion H^- due to motional effects as a function of time for the magnetic field $B = 1$ T. The inserts show typical trajectories corresponding to different parts of the anionic detachment curve.

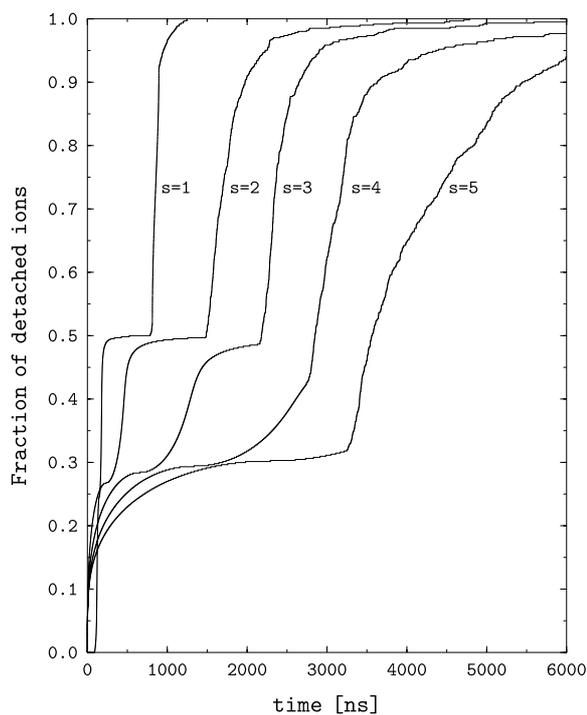


Figure 4. Fractions of detached trajectories, as a function of time, for Cs^- anions moving in a magnetic field $B = 1$ T. The initial ensembles of the anions correspond to the 5 lowest magnetically induced bound states, $s = 1-5$, of the infinitely heavy anion.

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