Landau quantization effects in ultracold atom–ion collisions

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Received 6 October 2011, in final form 24 October 2011
Published 18 November 2011
Online at stacks.iop.org/JPhysB/44/235201

Abstract
We study ultracold atom–ion collisions in the presence of an external magnetic field. At low collision energy the field can drastically modify the translational motion of the ion, which follows quantized cyclotron orbits. We present a rigorous theoretical approach for the calculation of quantum scattering amplitudes in these conditions. Collisions in different magnetic field regimes, identified by the size of the cyclotron radius with respect to the range of the interaction potential, are investigated. Our results are important in cases where use of a magnetic field to control the atom–ion collision dynamics is envisioned.

1. Introduction
The central role played by the collisional interaction in determining the macroscopic properties of cold atomic gases has motivated extensive theoretical and experimental studies of neutral atom collisions at very low collision energies over the last decade. For instance, magnetic Feshbach resonances have been discovered and theoretically analysed in several atomic species (see, e.g., [1, 2]). Such resonances allow the interatomic interaction to be finely tuned, and have been used to explore a variety of phenomena such as the BEC–BCS crossover [3] and strongly correlated quantum phases [4].

While atom–ion collisions at standard temperatures are a well-established subject [5], their behaviour at very low collision energy has only recently begun to raise a rapidly increasing interest. Atom–ion systems are in particular very promising candidates for the realization of collisional quantum gates [6] and for the study of ionic impurities in neutral Bose–Einstein condensates [7]. Experimental progress now makes ultracold atom–ion systems addressable in a controlled way [8]. First measurements of elastic cross sections and sympathetic cooling rates between a Bose condensed gas and a single ion held in a Paul trap have been reported in [8, 9]. Charge exchange has also been theoretically analysed both for its interest in fundamental molecular physics and in order to quantify harmful sources of atom loss or decoherence in the experiments [10, 11].

The presence of magnetically tuned Feshbach resonances induced by the hyperfine interaction has been demonstrated in free space [10]. Such resonances could in principle be engineered to increase the rapidity of collisional quantum gates or to manipulate the many-body properties of a neutral gas in the presence of a charged impurity [12]. However, non-trivial effects have to be taken into account to describe quantitatively atom–ion collisions in most non-idealized situations, such as trap confinement [13]. An additional feature neglected in previous work [10] is the influence of the magnetic field on the translational motion of the ion, which will classically follow helicoidal rather than rectilinear trajectories. Quantum mechanically, motion in the plane transverse to the field has to be quantized, resulting in the discretization of the continuum in Landau levels [14].

The dramatic influence of even a weak magnetic field on electron photodetachment was observed a long time ago [15] and modelled using a frame transformation approximation, which relies on the much smaller length scale of the interatomic potential compared to the cyclotron radius [16]. However, the frame transformation approach cannot be applied to ultracold atom–ion collisions since the typical length scales become comparable and therefore cannot be separated already at commonly used field intensities of a few hundred Gauss (see below). Numerically exact R-matrix calculations have been carried out for hydrogen photoionization but were limited to strong magnetic fields [17]. The main goal of our paper is to develop a rigorous theory applicable to atom–ion collisions in a magnetic field of arbitrary strength.

The paper is organized as follows. The system and general scattering properties in a magnetic field are introduced...
in section 2. Section 3 presents the numerical methods. Numerical results showing a variety of threshold, quantum interference and resonance phenomena are discussed in section 4. Concluding remarks and perspectives end this work.

2. Theoretical model

2.1. Background

We consider a low energy collision between a neutral atom with a singly charged ion in the presence of a uniform static magnetic field \( B \) oriented in the \( z \) direction. We suppose that both particles have spherical symmetry, vanishing internal spin, and that the atom has an infinite mass. The latter assumption allows the number of spatial degrees of freedom to be reduced from 6 to 3, thus avoiding complications related to the separation of the centre of mass motion [18]. Note that while this approximation prevents a quantitative comparison of our results with current experiments, light ions (Be+, Mg+,...) and heavy atoms (Rb, Cs, Sr, Yb,...) are customarily cooled down to ultracold temperatures. Experiments on mixed atom–ion systems using these species can in principle be envisioned, allowing our theory to be directly applied.

The spherically symmetric interparticle molecular potential \( V(\mathbf{r}) \) has a long-range behaviour determined by the second-order charge induced-dipole interaction \(-C_4 r^{-4}\), where \( 2C_4 \) is the static dipolar polarizability of the neutral atom. The detailed shape of the potential well is immaterial for ultracold collisions and it can be to excellent approximation described by energy-independent quantum defects or scattering lengths [13]. For this work we therefore take a simple model analytical form \( V(\mathbf{r}) = D_s (\chi^8 - 2\chi^{-4}) \) with \( x = r/r_s \). The s-wave scattering length \( a_s \) is currently unknown for any atom–ion system. Therefore, we perform some exploratory studies for different scattering lengths by adding a small correction to the bottom of the potential well to vary the value of \( a_s \) in the numerical calculations [19].

The Hamiltonian for a singly positively charged ion is

\[
H = \frac{(\mathbf{\hat{p}} - e\mathbf{A})^2}{2m} + V, \tag{1}
\]

where \( \mathbf{A} \) is the vector potential associated with \( \mathbf{B} \), \( \mathbf{\hat{p}} \) is the generalized momentum and \( e > 0 \) is the ion charge. The cylindrical symmetry about the direction of the magnetic field implies conservation of the axial projection \( L_z \) of the angular momentum \( \mathbf{\hat{L}} = \mathbf{\hat{r}} \times \mathbf{\hat{p}} \), whose quantized values will be noted \( h\Lambda \). It is convenient to choose the origin of the coordinates on the neutral atom and to work in the symmetric Landau gauge, in which the vector potential has the form \( \mathbf{A} = \frac{1}{2} \mathbf{B} \times \mathbf{r} \). With this choice, after some simple algebra in cylindrical coordinates \((\rho, \varphi, z)\) the Hamiltonian takes the following form:

\[
H = \frac{p_\rho^2}{2m} + \frac{p_z^2}{2m} + \frac{L_z^2}{2m\rho^2} + \frac{m\omega^2}{2}\rho^2 - \omega L_z + V, \tag{2}
\]

of a particle in a diamagnetic potential of Larmor angular frequency \( \omega = \frac{eB}{2m\rho^2} \) interacting with a fixed centre of force \( V \). The coordinate \( \rho \) is the distance from the \( z \) axis, \( p_\rho \) is its conjugate momentum and \( p_z \) is the linear momentum in the direction of \( \mathbf{B} \).

Conservation of the axial angular momentum reduces the orbital Zeeman term \( \omega L_z \) to a constant but its influence on the spectrum of \( H \) is essential. In fact, quantized energies for ion motion in the plane orthogonal to \( \mathbf{B} \), the Landau levels [14], can be expressed in terms of \( \Lambda \) and of the radial quantum number \( n \) by

\[
E_{n\Lambda} = \hbar \omega (2n + |\Lambda| - \Lambda + 1), \quad n = 0, 1, 2, \ldots \tag{3}
\]

Therefore, eigenvalues have infinite degeneracy, a quantum counterpart to the classical freedom to choose the cyclotron orbit centre keeping the energy fixed. The level spacing \( 2\hbar\omega \) for \( n \rightarrow n \pm 1 \) transitions corresponds to the energy of the classical cyclotron motion with angular frequency twice the Larmor frequency of precession, \( \omega_c = eB/m = 2\omega \).

The explicit expression of the eigenfunctions for planar motion with azimuthal angle \( \varphi \) is well known (see, e.g., [14]):

\[
\phi_{n\Lambda}(\rho, \varphi) = N_{n\Lambda} \frac{\rho}{\rho_0} J_{|\Lambda|}^{(2)} (\frac{\rho}{\rho_0}) e^{-\rho^2/2\rho_0^2}, \quad y = \frac{\rho}{\rho_0}, \tag{4}
\]

where \( \rho_0 = \sqrt{\hbar/m\omega} \) is the harmonic oscillator length and \( N_{n\Lambda} \) is a normalization constant. The quantum description of helicoidal motion is finally completed by a uniform translation in the \( z \) direction:

\[
\Phi^E_{n\Lambda}(\mathbf{r}) = \phi_{n\Lambda}(\rho, \varphi) \left| n\right> \left| e^{i\varphi}\right>, \tag{5}
\]

Note that to simplify the notation we have defined \( k_n = k_{n\Lambda} \) dropping the conserved quantum number \( \Lambda \) and of the radial quantum number \( n \) characteristic of the total energy \( E \) determines the magnitude of the longitudinal wave vector

\[
E = \frac{\hbar^2 k_n^2}{2m} + E_{n\Lambda}, \tag{6}
\]

where the first term on the rhs is the kinetic energy in the channel \( n, E_{\text{kin}} = \frac{\hbar^2 k_n^2}{2m} \).

Classically, as the atom and the ion approach, the spherically symmetric interaction distorts the cyclotron orbit modifying the energy distribution between longitudinal and transverse degrees of freedom. Quantum mechanically, a Landau collisional state \( \Phi^E_{n\Lambda} \) can be either reflected or transmitted across the collision centre with different probability amplitudes. In general, a collision starting with an initial quantum number \( n \) will populate all states \( \Phi^E_{n\Lambda} \) energetically accessible at energy \( E \) with a transition probability amplitude \( f_{\text{eq}} \). These energetically open channels are characterized by \( k_n^2 > 0 \), see equation (6). The closed channels \( k_n^2 < 0 \) are not energetically allowed at large atom–ion separation but can be populated during the collision giving rise to dramatic resonance effects.

Inspection of the typical length scales in the problem shows the essential role played by Landau quantization for cold atom–ion collisions. In the ultracold regime, the range of the interaction can be defined in terms of the polarizability coefficient \( C_4 \) through \( R^* = \sqrt{2mC_4R^2} \) [10]. The \( R^* \) parameter is proportional to the location \( R^*/\pi \) of the last node in the zero-energy wavefunction for infinite scattering length [19]. As such, it gives an estimate of the distance beyond which the wavefunction oscillates freely. The characteristic energy \( E^* = \hbar^2/l^2/(2mR^2) \) sets the scale at which quantum effects become important [20]. The quantum length scale
associated with cyclotron motion is \( a_{ho} \) which corresponds to the size of the lowest energy Landau state. The Landau level spacing is finally given by \( \hbar \omega_c \).

For a magnetic field intensity \( B \sim 10^5 \) G and typical values of \( C_4 \sim 10^2 \) au the range of the interaction becomes comparable to the harmonic oscillator length. Moreover, the transition between the weak \( R^* \ll a_{ho} \) and the strong field \( R^* \gg a_{ho} \) limits can be explored by varying \( B \) over an experimentally accessible range. The Landau splitting of the order of \( \mu K \) makes the discretized nature of the continuum in the magnetic field essential if collision energies of this order of magnitude are considered.

Taking into account Landau quantization, the scattering wavefunction takes the asymptotic behaviour

\[
\Psi_{n\Lambda}^E(\vec{r}) \rightarrow \Phi_{n\Lambda}^E(\vec{r}) + \sum_{k_n>0} f_{n\Lambda} (\text{sign}(z)k_n \leftarrow k_n) \Phi_{n\Lambda}^E(\rho, \varphi, |z|) \quad (7)
\]
in terms of an incoming \( \Phi_{n\Lambda}^E \) Landau state and of scattered waves outgoing in the open channels. One should note that since the transverse motion is confined by the magnetic field, scattering is effectively one dimensional. The measurable reflection and transmission coefficients for a progressive \( k_n > 0 \) incoming wave can be promptly identified from equation (7):

\[
R_{n\Lambda} = |f_{n\Lambda} (-k_n \leftarrow k_n)|^2, \quad T_{n\Lambda} = |\delta_{n\Lambda} + f_{n\Lambda} (k_n \leftarrow k_n)|^2. \quad (8)
\]

A different choice of the standardization of the wavefunction for \( |z| \rightarrow \infty \), the standing wave boundary conditions, will be more convenient for numerical calculations. In order to make explicit use of the invariance of the problem under the coordinate inversion \( \vec{r} \rightarrow -\vec{r} \) we first define new sets of reference functions in the \( z \) motion with well-defined behaviour under the \( z \rightarrow -z \) reflection \( \pi_z \). Namely, diagonal matrices of functions \( F^\pi \) and \( G^\pi \) regular and irregular at the origin are defined for open channels and parity \( \pi_z = \pm \) by

\[
\left\{ \begin{array}{l}
F^+_n(z) = k_n^{-1/2} \cos(k_nz) \\
F^-_n(z) = k_n^{-1/2} \sin(k_nz)
\end{array} \right. \quad \left\{ \begin{array}{l}
G^+_n(z) = k_n^{-1/2} \sin(k_n|z|) \\
G^-_n(z) = -k_n^{-1/2} \cos(k_nz).
\right. \quad (9)
\]

The corresponding reference functions for closed channels are

\[
\left\{ \begin{array}{l}
F^+_n(z) = \cos(k_nz) \\
F^-_n(z) = \sin(k_nz) \end{array} \right. \quad \left\{ \begin{array}{l}
G^+_n(z) = -\exp(-k_nz) \\
G^-_n(z) = -\exp(-k_n|z|).
\right. \quad (10)
\]

With these definitions, total parity of product functions \( \phi_{n\Lambda} F^\pi_m \) and \( \phi_{n\Lambda} G^\pi_m \) is \( \pi = \pi_z (\pm 1)^\Lambda \). We can now define a real reactance matrix \( K^\pi \) for each \( \pi_z = \pm \) and angular momentum \( \Lambda \) according to the asymptotic behaviour [21]

\[
\Psi_{n\Lambda}^E(\vec{r}) \rightarrow \Phi_{n\Lambda}^E(\vec{r}) + \sum_{n'} K^\pi_{n'\Lambda} \phi_{n'\Lambda}(\rho, \varphi) F^\pi_{n'}(z) \quad (11)
\]

If the transition matrix is also decomposed into symmetric and antisymmetric components \( f^\pi \),

\[
f^\pi_{n'\Lambda} (\text{sign}(z) k_n \leftarrow k_n) = f^+_{n'\Lambda} (E) + \text{sign}(z) f^-_{n'\Lambda} (E), \quad (12)
\]

the matrix relations

\[
f^\pi = iK^\pi (I - iK^\pi)^{-1} \quad (13)
\]

obtained comparing (7) and (11) can then be used to determine the \( f^\pi \) in terms of \( K^\pi \). Finally, we will make use of the unitary and symmetric scattering matrix, defined for the two parities as \( \Sigma^\pi = (I + iK^\pi) (I - iK^\pi)^{-1} \), below.

2.2. Wigner laws

The scattering quantities obey at low-energy Wigner laws, valid when the asymptotic de Broglie wavelength is much larger than the range of the effective potential in a given channel. Following [22], a collision channel in which the collision energy tends to zero will be termed new. Similarly to the 3D case, in which Wigner laws depend on the angular momentum quantum number, even in the present 1D configuration it is convenient to treat separately the \( \pi_z = \pm \) parity cases. An analysis along the lines of [22] gives the asymptotic behaviour

\[
f^\pi_{n'\Lambda} \sim -1 + O(k_n), \quad f^-_{n'\Lambda} \sim k_n, \quad (14)
\]

implying that for vanishing collision energy at the \( n \)th collision threshold a Landau state will be reflected with unit probability, irrespective of the value of \( \Lambda \). Moreover, the odd transition matrix element becomes negligible with respect to the even component, such that particles will be scattered with equal probability \(|f^\pi_{n\Lambda}|^2\) in forward and backward directions.

Inelastic processes consist in a transition to a Landau state of different transverse energy, and the corresponding scattering amplitudes obey for both parities the asymptotic law

\[
f^\pi_{n\Lambda} \sim \sqrt{k_n}, \quad (15)
\]

if \( n \) is new. The transition probability to a newly energetically accessible channel is then vanishing at threshold both in reflection and transmission. A similar relation

\[
f^\pm_{n\Lambda} \sim \sqrt{k_n'}, \quad (16)
\]

holds in the case where \( n' \) is new.

The Wigner laws allows one to define for positive parity an effective range-averaged potential \( V_{1D}(k_n) \) finite at threshold \( (k_n \rightarrow 0) \), which embeds the details of the short-range dynamics in a single parameter

\[
f^\pi_{n\Lambda} = \frac{1}{1 - \frac{h^2k_n^2}{2m\hbar^2}}. \quad (17)
\]

Such \( V_{1D}(k_n) \) can be used for instance to parametrize a 1D pseudopotential \( V_p \), i.e. a zero-range interaction \( V_p = g_{1D} \delta(z) \) which generates the same elastic scattering amplitude as the full problem at momentum \( k_n \). An associated one-dimensional scattering length can be defined for one open channel as the limit value \( a_{1D} = -\lim_{k_n \rightarrow 0} \eta(k) \), where \( \eta(k) \).
is the scattering phase shift extracted from the asymptotic wavefunction $\Psi_{\text{out}}^{E} (\vec{r}) \propto \sin(k|z| + \eta)\phi_{\text{out}} (\rho)$ [23]. Its relation with the scattering amplitude is
\[
a_{1D}^{\text{ID}} \propto \frac{\hbar\omega a_{\text{ho}}}{g_{1D}}. \tag{18}
\]
For a purely elastic collision $g_{1D}$ is real, otherwise its non-vanishing imaginary part accounts for inelastic loss processes. Note that unlike the three-dimensional case, where $g_{1D}$ is proportional to $g_{3D}$, here the scattering length is inversely proportional to the coupling constant. We will restrict most of our discussions to $g_{1D}$, since this is the quantity usually measured in experiments [24]. Moreover, pseudopotentials with coupling strength $g_{1D}$ are often used to model two-body interactions in many-body theories. A numerically exact approach for the determination of the scattering amplitude and hence of the coupling constant is the subject of section 3.

2.3. Feshbach resonances in quasi-1D

Feshbach resonance theory is well established for three-dimensional collisions. We shortly recall here its main elements in order to point out some differences with respect to the present quasi-one-dimensional configuration. For definiteness, let us focus on the case of one open channel and one isolated resonance. We will consider positive or negative parity scattering and drop the $\pi_\zeta$ parity label for notational convenience. A formal separation of background and resonant contributions to the scattering matrix can be performed following the standard Fano–Feshbach approach [25, 26]
\[
S = S_{bg} \frac{2(E - E_0 - \zeta_\xi) - i\gamma_\xi}{2(E - E_0 - \zeta_\xi) + i\gamma_\xi}, \tag{19}
\]
where $S_{bg}$ is the off-resonance scattering matrix, $E_0$ is the energy location of the molecular state responsible for the resonance, and $\zeta$ and $\gamma$ are the resonance shift and width, respectively. Near resonance the quantity $E_0$ typically presents a smooth linear dependence on the external parameters of the problem, the magnetic field or the potential depth in the present case.

At low momentum, according to the Wigner laws $S \sim (-1 - 2i\kappa a_{1D})$, $S_{bg} \sim (-1 - 2i\kappa a_{1D,bg})$, $\zeta_{\xi} \sim \text{const}$ and $\gamma_{\xi} \sim k$. Taking the $E \to 0$ limit, we obtain the resonantly modified $a_{1D}$ as
\[
a_{1D} = a_{1D,bg} \left(1 - \frac{\Delta}{E_0 + \zeta_0}\right), \tag{20}
\]
where we have defined $\Delta = \lim_{E \to 0} \gamma_{\xi}/(2\kappa a_{1D,bg})$. Note that on resonance ($E_0 = -\zeta_0$) the 1D scattering length diverges and according to (18) the system becomes non-interacting, $g_{1D} \to 0$ and the transmission coefficient tends to 1. This behaviour should be contrasted with the infinitely strong interaction obtained in three dimensions as the molecular state crosses the collision threshold. Note however that near resonance $a_{1D}$ will cross zero, and $g_{1D}$ will diverge, if $E_0 + \zeta_0 = \Delta$. With this remark, in the following we will refer to the divergence of the effective coupling constant as a zero-energy resonance situation.

3. Numerical methods

We solve our problem in the framework of the time-independent close coupling approach to potential scattering. In this method the full wavefunction is expanded in a suitable complete basis depending on a reduced set of coordinates. The choice of the basis function is inspired by the physics of the problem. Let us define a spherical system of coordinates $(r, \theta, \phi)$ with origin on the collision centre and polar axis in the $z$ direction. We identify an ‘inner region’ $r < R_0$ where the isotropic interatomic interaction initially dominates. The criterion for choosing the boundary $R_0$ is given below. In this internal region an expansion in spherical harmonics is used:
\[
\Psi_{\text{in}}^{E} (\vec{r}) = \sum_{\ell \geq 0} f_{\ell n}(r)Y_{\ell \zeta}(\theta, \phi), \tag{21}
\]
where the sum $\sum_{\ell \geq 0}$ runs only over even or odd values of $\ell$ for positive or negative parity, respectively. The coupled channel Schrödinger equation takes the form
\[
\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V + C - \Lambda_\zeta I\right] f(r) = EF(r). \tag{22}
\]
The effective centrifugal potential $V$ has a simple diagonal form with elements
\[
v_n(r) = \frac{\hbar^2(\ell(\ell + 1))}{2mr^2} + V(r), \tag{23}
\]
whereas the coupling matrix $C$ is formed by the matrix elements of the transverse oscillator potential
\[
C_{\ell \zeta} = \frac{m_\zeta \omega^2 r^2}{2} (Y_{\ell \zeta} | \sin^2(\theta)) (Y_{\ell \zeta}). \tag{24}
\]

Equation (22) is solved up to $R_0$ using the Johnson–Manolopoulos propagator [27], which computes the logarithmic derivative matrix $Z = ((\frac{d}{dr})^{-1})$ along a reaction coordinate using embedding propagators.

In the external $r > R_0$ region it is then natural to use cylindrical coordinates and an orthogonal basis of Landau oscillator states, equation (4):
\[
\Psi_{\text{out}}^{E} (\vec{r}) = \sum_{n} h_{n}(z)\phi_{n}^{\Lambda}(\rho, \psi). \tag{25}
\]
The coupled channel Schrödinger equation in the cylindrical basis becomes
\[
\left[-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + E_{\ell} + u\right] h(z) = E h(z). \tag{26}
\]
The diagonal matrix $E_{\ell}$ is composed by the Landau levels (3) and the coupling $u$ arises from the spherical atom–ion interaction $V$. In practice, we will always switch to the cylindrical representation at distances where the $V(r) = -C_1 r^{-4}$ asymptotic form is accurate. Moreover, in the same region the size of transverse oscillator states is much smaller than the radial coordinate $r$, such that a series expansion in the small parameter $a_{\text{ho}}/r$ can be performed. We find matrix elements
\[
u_{n \zeta} = \langle \phi_{n}^{\zeta} | V | \phi_{\zeta}^{\Lambda} \rangle = -\frac{C_4}{\zeta^4} \left(1 - \frac{2}{\zeta^2} \langle \phi_{n}^{\zeta} | \rho^2 | \phi_{\zeta}^{\Lambda} \rangle + \cdots \right). \tag{27}
\]
The second term in the expansion is rapidly decreasing \( \sim z^{-6} \) and in the present calculations we only retain lower order \( \sim z^{-4} \) diagonal coupling elements \( u_{nm} \) for both open and closed channels.

The representations (21) and (25) are matched on the spherical surface \( S_0 \) defined by \( r = R_0 \). We find that to ensure optimal numerical convergence one should choose \( R_0 \) in such a way that the relevant Landau states are localized in the two hemispheres without significant overlap on the equatorial plane\(^1\). The matching procedure is analogous to the one used in reactive scattering \([28, 29]\). We anticipate that the change from spherical to cylindrical geometry is at the origin of the peculiar scattering and resonance phenomena described in the next section.

In the external region \( r > R_0 \), we integrate equations (26) inwards from very large values of \( z \), with the asymptotic boundary condition (9)–(10) as a starting value. Let us denote the corresponding matrix solutions \( \tilde{F}^\pm \) and \( \tilde{G}^\pm \), which retain diagonal form due to the neglect of the off-diagonal elements in the coupling \( u \). The scattering solution is represented as

\[
\Psi_{n\Lambda}^\text{F}(|r\rangle) = \sum_{n'} C_{n'n}^\Lambda \phi_{n'} \phi_{n\Lambda}^\text{F} - d_{n'n}^\Lambda \phi_{n'} \phi_{n\Lambda}^\text{G},
\]

\[ r > R_0. \] (28)

Continuity of the scattering wavefunction and of its normal derivative on the spherical surface \( S_0 \) is used to determine \( \Lambda \) in terms of the logarithmic derivative matrix \( Z \).

The projection matrices

\[
\mathcal{F}_{n\Lambda} = \langle Y_{\Lambda} | \hat{F}_{n\Lambda} \phi_{n\Lambda} \rangle_{S_0},
\]

\[
\mathcal{F}_{n\Lambda}' = \langle Y_{\Lambda} | \frac{\partial}{\partial r} (\hat{F}_{n\Lambda} \phi_{n\Lambda}) \rangle_{S_0}
\] (29)

needed to this aim \([29]\) are numerically evaluated using Gauss–Legendre quadratures. Similar projection matrices \( \tilde{G}_{n\Lambda} \) and \( \tilde{G}_{n\Lambda}' \) involving the irregular reference functions are defined by replacing \( \hat{F} \) with \( \hat{G} \) on the rhs of (29). The reactance matrix is finally obtained for each parity using the equation \([29]\)

\[
\mathbf{K} = (Z G - G^T)^{-1} (Z F - F^T). \quad (30)
\]

4. Results and discussion

In this section, we apply our formalism to atom–ion diffusion with \( \Lambda = 0 \), a somewhat idealized situation to test our theoretical formalism which can however be in principle experimentally realized. For instance, instantaneous switching of a magnetic field in the propagation direction of an ion beam would project the plane wave describing the beam on a superposition of Landau states with different \( n \) and \( \Lambda = 0 \) without affecting the longitudinal momentum \( k \). A successive measurement of the transverse energy could be used to select the desired initial asymptotic state \( n \) for the collision.

While our calculations use a realistic model potential, previous work has shown that the short-range molecular physics can be accurately described in the ultracold regime by a single quantum defect parameter independent of energy

\(^1\) Typically, \( R_0 = 10 a_0 \) ensures a good convergence for collisions starting in the lowest Landau levels.
preexisting in free space. As such it can be termed a geometric resonance effect.

Interestingly, since in the weak-field limit the range of the potential can be neglected with respect to the transverse extension of the Landau state, the interaction $V$ can be expected to be well described by a zero-range 3D pseudopotential. With this approximation, equation (26) for $\Lambda = 0$ reduces to an analytically solvable model [23, 30]. The effective coupling constant of [23] is

$$\frac{g_{1D}}{\hbar \omega a_{ho}} = 2 \frac{a_s}{a_{ho}} \left( 1 + \frac{a_s}{a_{ho}} \zeta(1/2) \right)^{-1},$$

(32)

where $\zeta$ is the Riemann zeta function and $\zeta(1/2) = -1.46035$. The zero-order result $g_{1D} = 2a_s\hbar a_0$, obtained by neglecting the second term in the parenthesis on the rhs, simply represents the renormalization of $a_s$ obtained in the Born approximation by averaging the three-dimensional pseudopotential over the initial transverse Landau state. However, equation (32) also shows that a confinement-induced resonance arising from virtual excitations to asymptotically closed Landau states should appear for $a_s = -a_{ho}/\zeta(1/2) \simeq 0.6848a_{ho}$.

This non-trivial prediction is confirmed by the comparison with our numerical calculation shown in figure 1. The small shift in the resonance position can be understood by realizing that the result (32) is exact only in the limit of vanishingly small axial collision energy. However, when the atom and the ion are close together the relative energy $E$ in their unconfined 3D motion does not vanish but is rather equal to the zero-point energy $\hbar \omega$, see equation (3). This correction can be introduced by using an energy-dependent 3D pseudopotential [31], which replaces the zero-energy parameter $a_s$ with its finite energy counterpart $-\tan(\delta_{3D})/k_{3D}$. Here, $\delta_{3D}$ is the s-wave phase shift at energy $E$ and $k_{3D} = \sqrt{2mE/\hbar^2}$ is the wave vector in the three-dimensional motion. With this modification our numerical calculation becomes virtually identical to equation (32), thus confirming the accuracy of the pseudopotential approximation even for a long-range $r^{-4}$ potential under the appropriate conditions.

Since the zero-point energy is small with respect to the centrifugal barriers in equation (22), one can expect, as indeed proven by the agreement with the s wave model (32), that diffusion in partial waves $\ell > 0$ should be significantly suppressed. Our numerical approach allows us to check this property by a direct calculation. To this aim, we set $V = 0$ in the $v_{\ell>0}$ components of the interaction matrix $v$. The non-s-wave potentials are also turned off in the external region by using in the projection matrix elements (29) with $\ell > 0$ the unperturbed waves $F$ and $G$ in place of $\tilde{F}$ and $\tilde{G}$. Note that in spite of the fact that dynamically a single partial wave contributes to scattering, one cannot simply use a unique $\ell = 0$ in expansion (21), since a sufficient number of partial waves are in any instance cinematically necessary in order to represent the relevant Landau states on the spherical surface $S_0$ of radius $R_0$. The result of this purely s-wave calculation is not included in figure 1 as it is virtually indistinguishable from the exact result.

### Figure 2

Same as figure 1 but in the intermediate field case $a_{ho} = R^*$. The result of a purely s-wave calculation with the full molecular potential is also shown (see the text).

#### 4.2. Intermediate field regime

Let us now consider the variation of $g_{1D}$ with $a_s$ in the intermediate field regime $a_{ho} = R^*$ ($B \sim 10^3$ G). Like in weak-field conditions, a single geometric resonance is observed in the numerical simulation, see figure 2. The pseudopotential result in equation (32) in the energy-independent (I) and energy-dependent (II) formulations is only qualitatively correct. The purely s-wave calculation shows a significant shift in the resonance position from both the exact calculation and the pseudopotential models.

These findings can be rationalized as follows. The discrepancy between the pseudopotential and the purely s-wave result demonstrates the breakdown of the assumption of a zero-range potential, that is the importance of the long-range interplay between atom–ion and magnetic field potentials. The disagreement between the s-wave and the exact result is due to the important contribution of higher order partial waves. This contribution does not vanish even in the $k \to 0$ limit because of the zero-point energy. Its value ($\simeq 3 \mu K$), a factor $10^2$ larger than that in the weak-field case, and the long-range nature of the potential ensure that a few partial waves are scattered from the potential. More quantitatively, by artificially varying the number of partial waves as described above we find that a calculation restricted to $\ell = 0–4$ determines $g_{1D}$ with high accuracy. The good agreement in the resonance position between the exact result and the pseudopotential (I) approximation should be regarded as merely coincidental, stemming from the compensation of long-range and higher order partial waves effects.

#### 4.3. Strong field regime

Finally, figure 3 shows the behaviour of $g_{1D}$ for a strong field case $a_{ho} = 0.1R^*$, a tight confinement condition in which the potential range is larger than the Landau orbit radius. The required magnetic field intensity has an order of magnitude $B \sim 10^5$ G, a large yet experimentally attainable value. In this condition both the pseudopotential and the purely...
quantum defect on the horizontal axis is defined in terms of $R^*$ and is not shown. Note that for graphical purposes the normalized pseudopotential approximation breaks down in this situation is correctly reproduced by the numerical calculation but is extremely narrow, for $a_s = -R^*$ in particular.

$s$-wave model completely fail to reproduce the numerical results. Several zero-energy resonances are now available as $a_s$ (or $B$) is made to vary. The nature of such resonances can be understood from test calculations in which the atom–ion potential is suppressed in selected partial waves. Such calculations show that each broad feature in the tridimensional scattering length $a_s = ±R^*$ can in contrast be assigned to a single or few $\ell = 0–12$. That is, due to the relatively large zero-point energy ($\hbar \omega_c \simeq 300 \mu K$) the wavefunction picks up a significant phase shift at short range from different partial wave effective potentials. The narrowest features observed near $\xi = −1$ can in contrast be assigned to a single or few $\ell \geq 4$ angular momentum values, suggesting that most of the amplitude of the resonant bound state is localized in the potential well region. An analysis of the bound states of the systems will be needed to assign more precisely the features observed in the present scattering calculations.

4.4. Behaviour with collision energy

The zero-energy resonances described so far may shift as a function of the potential strength $a_s$ into the scattering continuum, giving rise to possible resonance effects observable as a function of collision energy. Let us consider in detail two potentials supporting 'typical' scattering lengths $a_s = ±R^*$ in the intermediate field case $a_{ho} = R^*$. Figure 4 shows the elastic reflection probability $R_{00}$ for a scattering event starting with the ion in the lowest Landau state $\phi_{00}$, as a function of collision energy. A decomposition of the scattering amplitude in even and odd components shows that the small value of the reflection coefficient $R_{00} = \frac{1}{|f_{00}^e|^2}$ between the $n = 0$ and $1$ thresholds is due to interference of parity amplitudes of relatively large magnitude, see figure 4. A similar situation has been reported for neutral atom scattering from short-range potentials in [32]. Figure 5 stresses the fact that the Wigner regime near the $n = 0$ threshold at which $R_{00} \rightarrow 1$ is correctly reproduced by the numerical calculation but is extremely narrow, for $a_s = -R^*$ in particular.

For $a_s = R^*$, a first peak at which $R_{00}$ reaches 1 is observed below the opening of the $n = 1$ level with energy $\hbar \omega_c$. This feature arises from the positive parity part $f^0$ of the scattering amplitude, and can be supposed to be a resonance arising from trapping of the ion in a long-lived superposition of excited Landau states.

To confirm the resonant character of this feature we calculate the time delay matrix introduced by Smith [33], defined for each parity as

$$Q^\gamma = i \hbar (S^\gamma) \frac{dS^\gamma}{dE}. \quad (33)$$

Note that $Q$ is expressed in terms of the open channel scattering matrix, such that its dimension equals the number of energetically accessible channels. The evolution with energy of the largest eigenvalue $q$ of the lifetime matrix can provide in particular information on the lifetime of the complex formed
during a collision. For instance, a narrow isolated resonance far from a collision threshold is characterized by a time delay following a familiar Lorentzian profile [33, 34]. In general, at very low collision energy threshold effects produce deviations from this simple picture making the analysis less direct [35].

In the present case the situation is simpler, since the lifetime origin. The long-lived isolated peaks are conclusively of resonant nature. Following a familiar Lorentzian profile [33, 34]. In general, at far from a collision threshold is characterized by a time delay during a collision. For instance, a narrow isolated resonance function of collision energy for the intermediate field case of figure 4. Only π, = + eigenvalues are shown. The long-lived isolated peaks are conclusively of resonant origin.

Below the second n = 1 and third n = 2 thresholds additional rapid variations with energy of smaller amplitude appear in \(R_{00}\). Again, the time delay analysis shown in figure 6 conclusively confirms the resonant nature of these features. The dispersive-like shape observed in the reflection probability arises from interference with background scattering, whereas the small modulation amplitude is explained by quenching due to \(n = 0 \rightarrow n' > 0\) inelastic processes.

Quite strikingly, such resonances seem to occur at similar locations with respect to each threshold. This property can be qualitatively interpreted using the pseudopotential analytical method of [36]. In this approach the resonance below the first threshold is assigned to a molecular state generated by the zero-range interaction in the \(n > 0\) subspace of closed channels. By a straightforward generalization consisting in replacing the shift operator \(A^j = \sum_n |\phi_{n+1,0}\rangle\langle\phi_{n,0}|\) below equation (10) of [36] by \(A^j = \sum_n |\phi_{n+m,0}\rangle\langle\phi_{n,0}|\), one can show that if a resonant state is present below the \(n = 1\) level there has to be a corresponding one below the \(mth\) threshold. Similar regularities in the Landau resonance spectrum have also been proved in low-energy electron photodetachment using a simplified model which assumes resonant states confined in the \(z = 0\) plane [37].
characteristic of zero-energy scattering has a finite energy counterpart. In fact, multiple resonance peaks are now observed between Landau thresholds. The narrowest features are most likely associated with bound states of relatively large \( \ell \) components. At variance with the intermediate-field case, a decomposition of the transition matrix identifies the resonance peaks as originating from both positive and negative parities. Cusp and rounded steps stemming from the non-analytical behaviour of the scattering matrix and from interference effects between parity components of the scattering amplitude are also visible near the opening of new energy thresholds.

5. Conclusions and outlook

In conclusion, we have presented a rigorous computational approach to study atom–ion collisions in the presence of a magnetic field. The weak-field case maps to a well-understood analytical model. In contrast, we have shown that a novel regime of strong confinement can be reached in atom–ion systems at experimentally attainable values of the magnetic field. A series of zero- and finite-energy resonances associated with high-order partial waves appears in this case. The resonance phenomena that we have analysed in this work should play an important role in applications based on magnetic control of the atom–ion dynamics.

In a forthcoming paper, we will present our results for the qualitatively different case of \(|A| > 0\) collisions and consider the case of a scattering centre not necessarily placed on the axis of the cyclotron orbit. In perspective, it will be interesting to investigate the interplay of pre-existing atom–ion magnetic Feshbach resonances and of Landau quantization. Moreover, in cases where the atom cannot be treated as infinitely massive, quasi-separability of the centre of mass motion might give rise to still unexplored resonance phenomena.

Acknowledgments

AS gratefully acknowledges support from CNRS and Rennes-Metropole.

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