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Abstract. Using the complex coordinate method, it is possible to compute the physical properties of atomic resonances above the ionization threshold. We show how to define and compute the electronic densities associated with these atomic resonances. The method is general and is illustrated for atomic Rydberg states in static and time-dependent external fields.

1. Introduction

For most purposes, a light atom can be accurately modelled by point particles interacting by a $1/r$ potential. Although atomic systems are in this sense *simple* systems, their dynamics can be very *complex*: classical phase space ($2N$ -dimensional) is typically divided into regions of regular and of stochastic (chaotic) motion, with the typical features of a fractal structure, involving all possible scales. Trajectories originating from a regular region of phase space are confined to N -dimensional submanifolds and can therefore be tracked over arbitrarily long times. This is no more possible for trajectories started from a stochastic region: the dynamics are chaotic and no prediction (even approximate) can be done on the long time behaviour of the system (characterized by the exponential divergence of trajectories with neighbouring initial conditions).

The simplest example is probably the helium atom, a three-body system which has a very complex classical dynamics (mostly chaotic) and, consequently, a complicated quantum spectrum, in the sense that it is not possible to obtain good quantum numbers and analytic expressions (even approximate) for all the energy levels. The same is true for the simplest atom, hydrogen, when an external electric and/or magnetic field is applied to it (Delande 1991).

One crucial property of atoms is that they can *ionize*. At sufficiently high energy—above the ionization threshold—the energy spectrum is continuous. For the hydrogen atom, the electron just escapes from the nuclear attraction and the continuum is structureless. However, it very often happens that a transient structure of the atom exists above the first ionization threshold, which ionizes after some finite time. In the quantum language, this is an *autoionizing* state or a *resonance* of the atom embedded in the continuum and can be characterized by its energy and its width. In an experimental spectrum like, for example, a photoionization cross section, it appears as a local structure emerging from a smooth background. Similar structures are observed in scattering experiments.

The appearance of resonances is in fact a very common situation in atomic physics, even in simple systems with few components, for example:

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(i) Above the first ionization threshold of the helium atom, when the two electrons are simultaneously excited, many resonances have been observed (Domke *et al* 1992). Near the second ionization threshold, they form series of doubly excited Rydberg states.

(ii) In the presence of a static electric field, an electron can tunnel through the Coulomb barrier and ionize, whatever its energy. Hence, strictly speaking, the spectrum of the hydrogen atom in a static electric field is a continuous one, and all bound states turn into resonances (Alvarez *et al* 1991).

(iii) The same is true for an external oscillatory electric field. The atom can ionize through a multiphoton transition, whatever the field strength and frequency. There are only resonances with finite lifetime (Casati *et al* 1988, Buchleitner and Delande 1993a).

In the presence of a static external magnetic field, the ionization threshold of a hydrogen atom is split into a series of Landau thresholds. There are true bound states, but also resonances (Delande 1991, Friedrich and Wintgen 1989, Hasegawa *et al* 1989).

Often, the physical properties of an atomic system are essentially dominated by the resonances. For example, the behaviour of an atom exposed to an intense laser field in a non-perturbative situation is dominated by its resonances. This is even more true for highly excited Rydberg (or double Rydberg) states of atoms, where the density of atomic resonances is very large. Beside their energies, all the other physical properties of the resonances are contained in their wavefunctions. The part of the wavefunction not too far from the nucleus contains the relevant information on the structure of the atomic state, while its behaviour at large distance mainly reflects the asymptotic properties of the Coulomb function, eventually perturbed by the external field (Grémaud *et al* 1993). This is why some important physical properties like the density of oscillator strengths or a localization phenomenon are insensitive to the long range behaviour, irrespective of whether a true bound state or a resonance is considered.

In this paper, we illustrate how the use of complex coordinates allows us to handle all aspects of atomic resonances—energies, widths, wavefunctions...—as easily as conventional treatments handle bound states. We will especially show that the calculation of the resonance wavefunction, although not obvious at first sight, is actually possible and illustrate this on specific systems. This is important for understanding the connection between classical and quantal dynamics in the semiclassical limit. As a matter of fact, it has been discovered in the last few years that, in a classically chaotic system, some wavefunctions of quantum bound states can be ‘scarred’ by classical periodic orbits, i.e. present an increased probability density in the immediate vicinity of some classical periodic orbits. The study of the scarring of the resonances is just beginning but of major importance for the understanding of quantum chaos in atomic and molecular systems (Delande 1991, Heller 1991). This paper is a step in this direction. It is organized as follows. In section 2, we recall the basic properties of the complex coordinate method. Section 3 is devoted to the calculation of the wavefunctions of resonances using this method. The technical and numerical aspects of its implementation for atomic resonances, which are essential to obtain physical converged results, are presented in section 4. Finally, in section 5, we illustrate the use of the method in various atomic systems, including time-dependent ones.

2. Complex coordinate method

The general idea of the complex coordinate method is to study the Green function of the system in the complex plane (Ho 1983, Chu 1978, Bhattacharya and Chu 1983, Maquet *et*

al 1983). If we consider a time-independent atomic system with Hamiltonian H , the Green function is defined as:

$$G(E) = \frac{1}{E - H} \quad (1)$$

for an arbitrary complex energy E .

$G(E)$ has a pole at the energy of each bound state, but also a cut along the real axis if the spectrum is continuous. The physical axis is the real energy axis, but the Green function on it depends on whether the real axis is approached from the upper or the lower complex half-plane. Thus, one defines two Green functions on the real axis:

$$G^{\pm}(E) = \frac{1}{E \pm i\eta - H} \quad (2)$$

where η is an arbitrary small positive number tending to 0 at the end of the calculation.

As will be shown below, any physical property of interest can be estimated from the Green function. A key property is that the energies of the resonances of the system are given by the positions of the complex poles of the analytic continuation of the Green function $G^+(E)$ beyond the real axis in the lower complex half-plane, the so-called second Riemann sheet. Of course, the analytic continuation of $G^-(E)$ in the upper half-plane has poles at the complex conjugate energies. In the scattering point of view, these complex poles coincide with the poles of the S -matrix (Smilansky 1991). The energy and the width of a resonance are related to the complex pole E_i through:

$$\begin{cases} \text{Energy} = \text{Re}E_i \\ \text{Width} = -2\text{Im}E_i. \end{cases} \quad (3)$$

The narrower the resonance, the closer the pole to the real axis. The complex poles are *not* eigenvalues of the Hamiltonian, because there is no physically acceptable solution of the Schrödinger equation for a complex energy. However, there is an unphysical solution—which exponentially diverges at large distance—which can be thought as the ‘wavefunction’ of the resonance (see Brandas and Elander (1989) for a discussion of these ‘Siebert’ or ‘Gamow’ states).

Using analyticity properties, the Green function on the real axis can be expressed as a function of the positions and residuals of its different poles.

In the complex coordinate method, the complex energies of the resonances can be obtained from a direct calculation (diagonalization of a complex operator). When the density of complex resonances is large, the Green function on the real physical axis is then obtained as a sum over all the resonances, which is more efficient (and also gives a much better physical picture) than computing directly the Green function on the real axis.

The first step is to consider the so-called complex rotated Hamiltonian of the system obtained from the usual Hamiltonian making the position and momentum complex (Ho 1983):

$$\begin{cases} r \rightarrow r e^{i\theta} \\ p \rightarrow p e^{-i\theta} \end{cases} \quad (4)$$

where θ is a real parameter called ‘rotation angle’. In this transformation, the canonical commutation relations between components of r and p are preserved.

Figure 1. Spectrum of the rotated Hamiltonian $H(\theta)$ (equation (6)) obtained from the Hamiltonian of the hydrogen atom in a magnetic field (equation (5)) through a dilation transformation $r \rightarrow re^{i\theta}$. The continua rotate around the Landau thresholds, exposing the resonances (crosses) as complex eigenvalues. $H(\theta)$ is truncated and diagonalized in a finite basis, and the continua appear as sets of discrete eigenvalues lying approximately on straight lines (diagonalization of a $25\,600 \times 25\,600$ complex symmetrical matrix: $\gamma = 0.1$; $L_z = 0$, odd parity spectrum; $\theta \approx 0.03$; $\alpha = 0.5$). The arrows indicate the successive Landau thresholds.

For the sake of simplicity, we apply the complex rotation method to the hydrogen atom exposed to an external magnetic field (Delande 1991, Friedrich and Wintgen 1989, Hasegawa *et al* 1989) (in section 5, we discuss how the method can be used in various atomic systems). Neglecting the finite mass of the nucleus and relativistic, QED... effects, the Hamiltonian writes, in atomic units:

$$H = \frac{1}{2}p^2 - \frac{1}{r} + \frac{1}{2}\gamma L_z + \frac{1}{8}\gamma^2(x^2 + y^2) \quad (5)$$

where γ denotes the magnetic field (along the z -axis) in atomic units of $B_c = 2.35 \times 10^5$ T and L_z the angular momentum along the z -axis. L_z and parity are good quantum numbers. In the following, we will study the ($L_z^\pi = 0^-$) series, although similar conclusions can be obtained for other series.

Applying the complex rotation, equation (3), to this Hamiltonian, we obtain:

$$H(\theta) = \frac{1}{2}p^2 e^{-2i\theta} - \frac{e^{-i\theta}}{r} + \frac{1}{2}\gamma L_z + \frac{1}{8}\gamma^2(x^2 + y^2)e^{2i\theta}. \quad (6)$$

If one defines the complex rotation operator:

$$R(\theta) = \exp\left(-\theta \frac{\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}}{2}\right) \quad (7)$$

the complex rotated Hamiltonian can be formally written as:

$$H(\theta) = R(\theta) H R(-\theta). \quad (8)$$

The rotated Hamiltonian $H(\theta)$ is clearly a *non-Hermitian* operator, whose spectrum is in general complex and depends on the rotation angle θ . The great property of the complex coordinate method is that the spectrum of $H(\theta)$ can be related to the resonances of the initial Hamiltonian H (Ho 1983). More precisely, the spectrum of $H(\theta)$ has the following properties, with reference to $H = H(\theta = 0)$ (see figure 1).

(i) The bound (discrete) spectra of $H(\theta)$ and H coincide below the first ionization threshold.

(ii) The continua are rotated by the angle 2θ into the lower half plane around their branching points.

(iii) The resonances of H coincide with the complex eigenvalues of $H(\theta)$. The real part (the energy) and the imaginary part (negative of the half width) are θ -independent, provided that the rotation of the continua has uncovered the resonances. The corresponding wavefunctions are square integrable.

In the specific case of the hydrogen atom in a magnetic field, there are multiple non-degenerate ionization thresholds at the different Landau levels:

$$E_n = (n + \frac{1}{2})\gamma \quad \text{with } n \text{ integer } \geq 0. \quad (9)$$

A typical (complex) spectrum of the rotated Hamiltonian is shown in figure 1. As expected, it displays bound states below the first threshold, rotated continua and resonances.

In a practical calculation, $H(\theta)$ is diagonalized in a basis of real, square integrable radial functions. For atomic systems with Coulomb interaction, a Sturmian basis (the basis of a discrete representation of the $SO(2, 2)$ dynamical group of the hydrogen atom) is well adapted to the dynamical symmetries of the problem. It is a *discrete* non-orthogonal basis which exactly takes into account the effect of the continuum (Clark and Taylor 1982, Delande and Gay 1984, 1986). In such a basis, each Sturmian state subsumes a part of the atomic continuum. As the basis is complete, it provides us with a fully exact representation of the atomic continuum, whatever the discrete-continuum and continuum-continuum interactions are.

In spherical coordinates (r, ϑ, φ) , the wavefunctions of the Sturmian states $|n\ell m\rangle^{(\alpha)}$ are (Halley *et al* 1993):

$$\begin{aligned} S_{n\ell m}^{\alpha}(r, \vartheta, \varphi) &= \langle r\vartheta\varphi | n\ell m \rangle^{(\alpha)} \\ &= \left(\frac{(n-\ell-1)!}{(n+\ell)!} \right)^{1/2} \left(\frac{2r}{\alpha} \right)^{\ell} e^{-r/\alpha} L_{n-\ell-1}^{(2\ell+1)} \left(\frac{2r}{\alpha} \right) Y_{\ell m}(\vartheta, \varphi) \end{aligned} \quad (10)$$

with $|m| \leq \ell < n$, where $L_{n-\ell-1}^{(2\ell+1)}$ are associated Laguerre polynomials and $Y_{\ell m}(\vartheta, \varphi)$ the usual spherical harmonics. For any positive value of the parameter α , the Sturmian basis set is complete and orthonormalized for an unusual scalar product, involving a $1/r$ additional element (Delande 1991). Because of this non-orthogonality, when written in a Sturmian basis, the Schrödinger equation does not correspond to a usual eigenvalue problem, but rather to a generalized one of the type:

$$(A - E_i B) \cdot x_i = 0 \quad (11)$$

where A and B are two fixed matrices, E_i and x_i the generalized eigenvalues (i.e. energies) and eigenvectors, respectively.

One advantage of the Sturmian basis is that the different operators in the Hamiltonian have strong selection rules on the three quantum numbers n , ℓ and m . The matrices involved are consequently sparse, allowing the use of an efficient diagonalization algorithm. The matrix representing the unrotated Hamiltonian H in the Sturmian basis is real symmetric. Because only the radial variable r —and *not* the angular variables ϑ, φ —is affected by the complex rotation, the generalized eigenvalue problem for the complex rotated Hamiltonian $H(\theta)$ involves sparse *complex symmetric* matrices (*not* complex Hermitian matrices) (Delande *et al* 1991, Grémaud *et al* 1993, Halley *et al* 1993).

The properties of complex rotated operators depend on which Hilbert space they act in. For example, $R(\theta)$ transforms an outgoing spherical wave e^{ikr} (not square integrable) to an exponentially decreasing (square integrable) outgoing wave $e^{ikr \cos \theta} e^{-kr \sin \theta}$. This is why the resonances, which are unphysical solutions of the original Schrödinger equation, can be mapped onto square integrable eigenfunctions of the complex rotated Hamiltonian. In contrast, an ingoing wave is transformed to an exponentially increasing ingoing wave, which is not an acceptable physical solution. Consequently, one has to be careful when using formal equations as equation (8) and keep in mind the type of functions on which the complex rotation operator acts (Ho 1983).

From the mathematical point of view, the complex coordinate method is far from obvious and relies on a subtle analysis of the analyticity properties of the Hamiltonian and Green function, far beyond the aim of this paper; for mathematical details, see Ho (1983) and Balslev and Combes (1971). It can be applied to 'dilation analytic' Hamiltonians. These include not only the static magnetic field, but also the static and oscillatory electric field and the many-body Coulomb problem, where it was first studied (an important example are the autoionizing double excited states of the helium atom, see Wintgen and Delande (1993)).

The complex coordinate method is not only able to give directly the (complex) energies of the resonances, but also any physical property of interest. It can be shown (Johnson and Reinhardt 1983) that the Green function of the rotated Hamiltonian is simply related to the original Green function of the unrotated Hamiltonian through:

$$G(E) = \frac{1}{E - H} = R(-\theta) G_\theta(E) R(\theta) = R(-\theta) \frac{1}{E - H(\theta)} R(\theta). \quad (12)$$

Compared to the original Green function, the Green function of the rotated Hamiltonian does not have any singularity on the real axis. It has a smooth continuation in the lower complex half-plane down to the rotated continua. In other words, the complex dilation, by rotating the continua in the complex plane, allows one to obtain *directly* the analytic continuation of the Green function and consequently the resonances. For $\theta > 0$ (respectively $\theta < 0$), the rotated Green function is the analytic continuation of $G^+(E)$ (respectively $G^-(E)$). When using equation (12), one must take care to apply this expression on both sides on square integrable functions.

As an example, equation (12) makes it possible to compute easily the photoionization cross section from a bound state (Delande *et al* 1991, Iu *et al* 1991). If $|g\rangle$ denotes the initial bound state (with energy E_g) and $T = e \cdot r$ the dipole operator (depending on the light polarization e), the Fermi Golden rule gives the photoionization cross section as:

$$\sigma(\omega) = \frac{4\pi^2\omega}{c} |\langle \phi_E | T | g \rangle|^2 \quad (13)$$

where $|\phi_E\rangle$ is the continuum eigenstate of energy $E = E_g + \hbar\omega$ normalized per unit energy.

If there is more than one eigenstate of energy E (degenerate continua above the second ionization threshold), a sum over continuum eigenstates has to be added in equation (13). The projection onto the subspace of energy E is directly related to the cut of the Green function along the real axis. Indeed, one has for a non-degenerate continuum:

$$|\phi_E\rangle \langle \phi_E| = \frac{1}{2i\pi} (G^-(E) - G^+(E)). \quad (14)$$

Using the representation of the Green function (12), one gets ($\theta > 0$):

$$|\phi_E\rangle \langle \phi_E| = \frac{1}{2i\pi} \left[R(-\theta) \frac{1}{H(\theta) - E} R(\theta) - R(\theta) \frac{1}{H(-\theta) - E} R(-\theta) \right] \quad (15)$$

The eigenstates of $H(\theta)$ are normalized for the scalar product for complex symmetric matrices:

$$H(\theta)|\psi_{i\theta}\rangle = E_{i\theta}|\psi_{i\theta}\rangle \quad \langle\bar{\psi}_{j\theta}|\psi_{i\theta}\rangle = \delta_{ij} \quad (16)$$

where $\langle\bar{\psi}|$ denotes the complex conjugate of $\langle\psi|$ in the Sturmian basis, i.e. the transpose of $|\psi\rangle$. They also satisfy the following closure relation:

$$\sum_i |\psi_{i\theta}\rangle \langle\bar{\psi}_{i\theta}| = 1. \quad (17)$$

The Green function of the rotated Hamiltonian is extremely simple in the eigenbasis:

$$G_\theta(E) = \frac{1}{E - H(\theta)} = \sum_i \frac{|\psi_{i\theta}\rangle \langle\bar{\psi}_{i\theta}|}{E - E_{i\theta}}. \quad (18)$$

Because the rotated continua and the poles lie in the lower half-plane, equation (18) is now free of any divergence along the real positive axis and allows for a safe calculation of any physical relevant quantity, for example the photoionization cross section (see equations (13) and (15)). Changing θ to $-\theta$ is equivalent to changing $H(\theta)$ into its complex conjugate:

$$\begin{cases} E_{i,-\theta} = \overline{E_{i,\theta}} \\ |\psi_{i,-\theta}\rangle = |\bar{\psi}_{i,\theta}\rangle. \end{cases} \quad (19)$$

Hence, equation (15) becomes, with equation (18):

$$|\phi_E\rangle \langle\phi_E| = \frac{1}{2i\pi} \sum_i \left[\frac{R(-\theta)|\psi_{i\theta}\rangle \langle\bar{\psi}_{i\theta}| R(\theta)}{E_{i\theta} - E} - \frac{R(\theta)|\bar{\psi}_{i\theta}\rangle \langle\psi_{i\theta}| R(-\theta)}{\overline{E_{i\theta}} - E} \right]. \quad (20)$$

This equation, combined with equation (13), gives the photoionization cross section:

$$\sigma(\omega) = \frac{2\pi\omega}{ic} \sum_i \left[\frac{\langle g|T R(-\theta)|\psi_{i\theta}\rangle \langle\bar{\psi}_{i\theta}| R(\theta) T|g\rangle}{E_{i\theta} - E_g - \hbar\omega} - \frac{\langle g|T R(\theta)|\bar{\psi}_{i\theta}\rangle \langle\psi_{i\theta}| R(-\theta) T|g\rangle}{\overline{E_{i\theta}} - E_g - \hbar\omega} \right]. \quad (21)$$

The last equation is somewhat formal in the sense that some matrix elements are formally defined. $T|g\rangle$ having a real radial wavefunction exponentially decreasing at infinity and localized around the nucleus, $R(\theta)T|g\rangle$ is well defined and square integrable, which makes the matrix element $\langle\bar{\psi}_{i\theta}|R(\theta) T|g\rangle$ meaningful. In contrast, $R(-\theta)|\psi_{i\theta}\rangle$ is not a well defined state (it is actually exponentially increasing at infinity) and the matrix element $\langle g|T R(-\theta)|\psi_{i\theta}\rangle$ has in fact to be understood as $\langle\bar{\psi}_{i\theta}|R(\theta) T|g\rangle$, which coincides with $\langle\bar{\psi}_{i\theta}|R(\theta)T|g\rangle$, for an initial state with a real radial wavefunction. The corresponding expression for the second term leads naturally to the complex conjugate expression. The final result is:

$$\sigma(\omega) = \frac{4\pi\omega}{c} \operatorname{Im} \sum_i \frac{\langle\bar{\psi}_{i\theta}|R(\theta) T|g\rangle^2}{E_{i\theta} - E_g - \hbar\omega}. \quad (22)$$

The complex coordinate method ensures automatically that the cross section is real, but not that it is a positive quantity! Indeed, from equation (22), the cross section appears as

a sum over all resonances. The contribution of each resonance is a Beutler–Fano profile (Fano 1961) whose shape parameter is:

$$q = -\frac{\operatorname{Re}(\overline{\psi_{i\theta}}|R(\theta) T|g\rangle)}{\operatorname{Im}(\overline{\psi_{i\theta}}|R(\theta) T|g\rangle)}. \quad (23)$$

An individual contribution can be either positive or negative. Furthermore, each of them has in general to be negative at some energy. It is only the sum over all resonances which is a physical quantity and has to be positive for any energy. Once a given resonance is uncovered by the rotation of the continua, the energy $E_{i\theta}$ is in fact independent of θ , and the same is true for the matrix element $\langle\overline{\psi_{i\theta}}|R(\theta) T|g\rangle$. This means that the complex coordinate method, although formally depending on the parameter θ , reveals in fact the underlying nature of the Green function.

In a practical calculation, the Sturmian basis is truncated in order to have finite matrices to diagonalize. Consequently, the basis set is no longer complete. However, both discrete states and isolated resonances are represented by square integrable eigenstates of the rotated Hamiltonian and can be found efficiently if a large enough basis set is used. The stability of the complex energies with respect to a change of the basis size, the parameter α of the Sturmian basis and the rotation angle θ can be easily checked. On the contrary, the rotated atomic continua cannot be obtained from the diagonalization of a finite matrix: they are replaced by sets of discrete eigenvalues approximately lying on the half-lines representing the rotated continua. The interaction between continua is ‘automatically’ taken into account through the interaction between these discretized quasi-continua. The individual complex energies in these sets and the associated matrix elements are not converged, as they vary with the size of the basis and with the α and θ parameters. However, provided they are sufficiently dense (i.e., when the size of the basis is sufficiently large, such that $|\operatorname{Re}(E_{i,\theta} - E_{i+1,\theta})| \ll |\operatorname{Im}(E_{i,\theta})|$ for two consecutive states of the rotated continuum), they mimic the true continua and the global effect of the quasi-continuum is well converged. It gives a smooth background in the photoionization cross section which is essential to obtain a positive result.

The calculation of the cross section requires computation of matrix elements like $\langle\overline{\psi_{i\theta}}|R(\theta)T|g\rangle$, where $|\psi_{i\theta}\rangle$ is obtained by the numerical diagonalization and appears as a linear combination of Sturmian functions. Because the complex rotation acts only on the radial coordinate, the angular part of the matrix element does not change when complex coordinates are used. The selection rules follow from those of the transition operator T , for example $\Delta m = 0$, $\Delta \ell = \pm 1$, for a linear polarization along the quantization axis. The evaluation of the radial matrix elements is easy using the dynamical group $SO(2, 2)$ of the hydrogen atom and involves simple algebraic expressions known analytically (Delande and Gay 1984). As the initial state $|g\rangle$ is itself obtained as a *real* dilation acting on a Sturmian function, one is left with the evaluation of the matrix elements of a *complex* dilation (i.e. with non-zero real and imaginary components) in the Sturmian basis. This is obtained again from group theory, since the generator of the dilation $(\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r})/2$ belongs to the $SO(2, 2)$ Lie algebra. The result is:

$$\begin{aligned} & {}^{(a)}\langle n\ell m|\exp(\tfrac{1}{2}i\eta\mathbf{r} \cdot \mathbf{p} + \mathbf{r} \cdot \mathbf{p})|n'\ell m\rangle^{(a)} \\ &= \frac{(-1)^{n-\ell-1}}{(2\ell+1)!} \frac{1}{(\cosh \tfrac{1}{2}\eta)^{2\ell+1}} (\tanh \tfrac{1}{2}\eta)^{n+n'} \left[\frac{(n+\ell)!(n'+\ell)!}{(n-\ell-1)!(n'-\ell-1)!} \right]^{1/2} \\ &\quad \times F \left[-n+\ell+1, -n'+\ell+1, 2\ell+2; -\frac{1}{\sinh^2 \tfrac{1}{2}\eta} \right] \end{aligned} \quad (24)$$

where $F[a, b, c; d]$ is the hypergeometric function (Abramowitz and Stegun 1965) and η any complex number.

3. Calculation of the wavefunctions

The calculation of the wavefunctions follows the same lines as the calculation of the cross section described above. Indeed, equation (20) gives the eigenstate of the physical problem at real energy as an expression involving only the eigenstates of the rotated Hamiltonian. By projecting this equation onto configuration space, one obtains the electronic density at real energy E , that is the continuum states of the atom:

$$|\phi_E(r)|^2 = \frac{1}{2i\pi} \sum_i \left[\frac{\langle r | R(-\theta) | \psi_{i\theta} \rangle \langle \bar{\psi}_{i\theta} | R(\theta) | r \rangle}{E_{i\theta} - E} - \frac{\langle r | R(\theta) | \bar{\psi}_{i\theta} \rangle \langle \psi_{i\theta} | R(-\theta) | r \rangle}{\bar{E}_{i\theta} - E} \right] \quad (25)$$

which can be further reduced to:

$$|\phi_E(r)|^2 = \frac{1}{\pi} \operatorname{Im} \sum_i \frac{\langle r | R(-\theta) | \psi_{i\theta} \rangle^2}{E_{i\theta} - E}. \quad (26)$$

Here, again, great care is needed when evaluating matrix elements like $\langle r | R(-\theta) | \psi_{i\theta} \rangle$ because $|r\rangle$ is not a square integrable function. The state $R(-\theta) | \psi_{i\theta} \rangle$ is not well defined: it is formally a solution of the Schrödinger equation of the unrotated Hamiltonian for the complex energy $E_{i\theta}$. Hence, it cannot be a square integrable function. As discussed above, it is rather an exponentially increasing function at large radius r . Equivalently, $\langle r | R(-\theta)$ can be thought of as the 'complex' bra $\langle r e^{i\theta} |$. The matrix element $\langle r | R(-\theta) | \psi_{i\theta} \rangle$ then appears as the wavefunction of the well-defined square integrable rotated state $|\psi_{i\theta}\rangle$ computed at the complex position $r e^{i\theta}$:

$$|\phi_E(r)|^2 = \frac{1}{\pi} \operatorname{Im} \sum_i \frac{(\psi_{i\theta}(r e^{i\theta}))^2}{E_{i\theta} - E}. \quad (27)$$

The electronic density at energy E appears as a sum over all the resonances weighted by the factor $1/(E - E_{i\theta})$. This is completely analogous to equation (22) for the cross section. The sum (27) is an exact result: all the intricate features of the discrete-discrete, discrete-continuum and continuum-continuum interaction are contained in the complex-valued spectrum of the rotated Hamiltonian.

In the sum (27), nothing ensures *a priori* that the electronic density is positive. Indeed, as for the cross section, contributions of individual resonances can be negative, it is only the sum over all the resonances which is positive. However, for an isolated resonance—lying much closer to the real axis than to the other resonances, $|\operatorname{Im} E_{i\theta}| \ll |E_{i\theta} - E_{j\theta}|$ —the sum in equation (27) is dominated by a single term and the electronic density at energy $E = \operatorname{Re}(E_{i\theta})$ is simply:

$$|\phi_{E=\operatorname{Re}(E_{i\theta})}(r)|^2 \simeq |\psi_i(r)|^2 \equiv \frac{1}{\pi |\operatorname{Im} E_{i\theta}|} \operatorname{Re} (\psi_{i\theta}(r e^{i\theta}))^2. \quad (28)$$

This equation makes it possible to define $\operatorname{Re} (\psi_{i\theta}(r e^{i\theta}))^2$ as the (unnormalized) electronic density of the atomic resonance. It has the following important properties.

(i) It is a real, well defined quantity.

(ii) Provided the rotation angle is sufficiently large so that the resonance is uncovered, it is *independent* of the rotation angle θ . The rotation of the θ -dependent eigenstate $|\psi_{i\theta}\rangle$ is compensated for by the 'backward' rotation $\langle r|R(-\theta)$ of the spatial coordinate. This is in contrast with the simple wavefunction $\psi_{i\theta}(r)$ of the rotated eigenstate, which depends on θ and has no clear physical meaning.

(iii) The price to pay for the preceding crucial property is that the wavefunction of the resonance $\psi_{i\theta}(r e^{i\theta})$ is not square integrable and even exponentially divergent at large distances.

(iv) For an exactly bound state (below the first ionization threshold), this definition coincides with the usual one.

(v) For an isolated resonance, the electronic density is mainly positive.

(vi) For overlapping resonances, the physical electronic density (on the real energy axis) is a complicated mixture of the various resonances. The electronic densities for individual resonances possibly have simpler structures, at the price of having eventually large negative values.

Figure 2. Electronic density of the resonance with complex energy $0.13107 - i0.99 \times 10^{-3}$ au for the hydrogen atom in a magnetic field (data as in figure 1; this resonance is marked with a circle), obtained from equation (28), plotted in the (ρ, z) plane containing the magnetic field axis. The full line contours (respectively broken) show the constant positive (respectively negative) values of the electronic density. (a): z from -70 to $+70$ au, ρ from -35 to $+35$ au; the electronic density is mainly positive and displays the structure of the individual resonance. (b): z from 60 to 100 au, ρ from -20 to $+20$ au. In the magnetic field direction where ionization takes place, the electronic density of this individual resonance has oscillations between positive and negative values.

This is illustrated in figures 2 and 3. In figure 2, we show the wavefunction of an individual resonance for the hydrogen atom in a magnetic field (this is one of the resonances visible in the spectrum of figure 1). This resonance is relatively well isolated and its electronic density is mainly positive. The minimum (negative) value is about -20% of the

Figure 3. Electronic density of the non-degenerate continuum eigenstate at real energy 0.131 07 for the hydrogen atom in a magnetic field (data as in figure 1), obtained from equation (27) as a sum over all the resonances, plotted in the (ρ, z) plane containing the magnetic field axis. The contours show the constant positive values of the electronic density (negative values are 20 times smaller than in figure 2). (a): z from -70 to $+70$ au, ρ from -35 to $+35$ au; the electronic density is very similar to the one of the individual resonance in figure 2. This shows that the atomic continuum at this energy is dominated by a single resonance. (b): z from 60 to 100 au, ρ from -20 to $+20$ au; in the magnetic field direction where ionization takes place, the electronic density has oscillations, but remains positive. The smooth background due to the set of other resonances adds to the oscillations in figure 2(b) to give a physically acceptable positive electronic density.

maximum value. It is essentially far in the z -direction—where ionization takes place—that large negative values are obtained. There, the Hamiltonian is quasi-separable in cylindrical coordinates: the physical picture is an electron in the first bound Landau level in the transverse direction ρ and in a free state along the z -axis. This structure is already visible in the individual resonance in figure 2(b), although the negative (broken lines) and positive (full lines) values of the electronic density are almost equal in magnitude.

The full electronic density at the corresponding energy on the real axis is plotted in figure 3. It is obtained by the sum over all resonances, see equation (27). As expected, it is positive everywhere, even far in the z -direction (because of the unavoidable truncation of the infinite sum in equation (27), there are tiny negative regions with a magnitude of less than 1% of the maximum). The negative contribution of the main resonance is compensated by the total effect of the other resonances, including the quasi-continua. Far in the z -direction, the latter give a smooth positive background which almost exactly compensated the positive and negative oscillations of the main resonance, see figure 3(b) and compare with figure 2(b). Clearly, the general structures in figures 2(a) and 3(a) are very similar, which proves that the continuum is dominated by the individual resonances (Grémaud *et al* 1993).

It should be emphasized that the appearance of negative electronic densities for individual resonances is *not* due to unconverged calculations. It is an intrinsic property of the complex coordinate method. For the figures 2 and 3, the basis set is sufficiently large

for the electronic densities to be very well converged (better than 0.1% of the maximum, which is not visible at the scale of the figures).

4. Numerical implementation

Although equations (26)–(28) define the various wavefunctions to compute, the practical calculation is somewhat tricky. Indeed, the result of the numerical diagonalization of the rotated Hamiltonian in a Sturmian basis is a set of square integrable rotated eigenstates. The wavefunctions $\psi_{i\theta}(\mathbf{r})$ of these rotated resonances decrease exponentially at large distance and are accurately obtained as linear combinations of the Sturmian functions. However, this does not allow for an accurate computation for a complex position $\mathbf{r}e^{i\theta}$. The difficulty is comparable to obtaining the value of an analytic function everywhere in the complex plane from the knowledge of its values on the real axis: although there is in principle a unique solution, the fact that the solution is known only numerically on the real axis makes the extrapolation difficult.

This can also be seen directly from the Sturmian functions themselves. These are the products of polynomials of the radial coordinate r by a decreasing exponential: their values everywhere in the complex plane can be extremely easily computed. However, all the zeroes of the Laguerre polynomials lie on the positive real axis. Therefore, on the real axis, the Sturmian functions have an oscillatory structure, but, outside this axis, they may take much larger complex values. The contributions of very excited Sturmian functions (above the maximum n value at which the basis is truncated) to the ‘exact’ eigenstate may be negligible along the real r -axis, but important for a complex radial coordinate. Consequently, we have found that the direct use of equations (27) or (28) is not possible, except for resonances with very small widths and for small rotation angles (Grémaud *et al* 1993).

A better strategy is to come back to the expression (26). There, the expansion of $\psi_{i\theta}$ in the Sturmian basis is directly obtained by the numerical diagonalization. As the matrix elements of the complex dilation operator $R(-\theta)$ in the complete Sturmian basis are known in analytic form, see equation (24), one can deduce the expansion of $R(-\theta)|\psi_{i\theta}\rangle$ in the Sturmian basis and from there the electronic density. The advantage is that one needs to evaluate the Sturmian functions only at real values of the radial coordinates which gets rid of the previous divergence. The price to pay is the divergence of the coefficients of the expansion in the Sturmian basis. Indeed, the matrix elements of the complex dilation operator $R(\theta)$ diverge at large n (remember that this is not a unitary operator). Roughly, the diagonal element $\langle n\ell m | R(\theta) | n\ell m \rangle$ scales as $e^{n\theta}$: the effect of the truncation of the basis at large n is thus amplified considerably. However, we have observed that this is a ‘local effect’ which spoils only the higher components of the expansion. Roughly, the generic behaviour of the coefficients of the expansion in the Sturmian basis is the following: if $n_{\max}$ is the maximum n value used in a diagonalization, the coefficients for $|\psi_{i\theta}\rangle$ are of course very small just below $n_{\max}$ if the calculation is converged. The coefficients for $R(-\theta)|\psi_{i\theta}\rangle$ are slowly decreasing at large n , except in the immediate vicinity of $n_{\max}$ where they can take extremely large unphysical values. Hence, a second truncation of the expansion slightly below $n_{\max}$ leads to a well converged resonance wavefunction. Typically, truncating at $n = n_{\max}e^{-2\theta}$ or below is enough. This second truncation is definitely unavoidable if one thinks that the strategy is to try to represent as much as possible of the *non-normalizable* resonance wavefunction with *exponentially decreasing* Sturmian functions. For all practical purposes, this strategy has been found easy to implement and efficient. All the electronic

densities plotted in this paper have been obtained using this method. This difficulty exists for computing the wavefunctions of individual resonances, equation (28). It is therefore not related to the effect of the rotated quasi-continua. Indeed, we have checked, in the case of a pure electric field where there are no longer any rotated continua but only isolated resonances, that the same problem remains.

5. Extension to other atomic problems

For simplicity, we have considered in the previous sections the hydrogen atom in a magnetic field below the second ionization threshold, so that the Hamiltonian is time-independent and non-degenerate. The conclusions obtained are nevertheless very general.

When there are multiple continua, the continuum states are degenerate (this is for example the case for the hydrogen atom in a magnetic field above the second ionization threshold, or for the helium atom above the first ionization threshold). There is no longer a single continuum state $|\phi_E\rangle$, but a set of degenerate continuum states. However, the preceding analysis remains entirely valid, just with the replacement of $|\phi_E\rangle\langle\phi_E|$ in equations (20) by the projector onto the whole subspace of energy E (continuum-continuum interaction is exactly taken into account by the complex coordinate method if a complete discrete basis set is used). What is obtained for the electronic density, equations (26) and (27), is just summed over this subspace. If a well defined state is to be studied in this degenerate subspace, an additional projector (specifying, for example, the asymptotic behaviour of the wavefunction) has to be added on both sides of the Green function in equation (12). The important point is that, even for infinitely degenerate continua, the individual resonances remain non-degenerate and consequently have a well defined electronic density, equation (28), as in the simple case previously discussed.

When the external potential is not binding, all states turn into resonances and the continua disappear (they have no branch point to turn around). This is for example the case for the hydrogen atom in a static external electric field (Alvarez *et al* 1991) or in combined static electric and magnetic fields (Main and Wunner 1992). Usually, the energy spectrum of the unrotated Hamiltonian is the full real axis with infinite degeneracy. The situation is basically not changed for the rotated Hamiltonian, the rotated continua being simply replaced by a discrete set of resonances lying far from the real axis.

Multi-electronic systems, like the helium atom, can be treated as well. The key point is to use a complete discrete basis to numerically diagonalize the complex rotated Hamiltonian. This has been done for the helium atom with the perimetric coordinates and Sturmian-like basis functions. The method described in the present paper should allow for the computation of wavefunctions and electronic densities of the various autoionizing resonances (not only the very narrow ones as in Richter *et al* (1992)).

Another possible extension of the method is to the calculation of electronic densities in other representations, for example in momentum space or in phase space using Husimi distributions. The latter involves projection of equation (20) onto coherent states $|\Omega\rangle$ (Delande 1988, Buchleitner 1993). The only amendment to the previous equations is that these states do not have real radial wavefunctions, yielding the equation (Buchleitner and Delande 1994):

$$|\langle\Omega|\phi_E\rangle|^2 = \frac{1}{\pi} \text{Im} \sum_i \frac{\langle\bar{\psi}_{i0}|R(\theta)|\Omega\rangle\langle\bar{\psi}_{i0}|R(\theta)|\bar{\Omega}\rangle}{E_{i0} - E}. \quad (29)$$

If only one term is retained in the sum, one obtains the Husimi distribution of a resonance, which again can be negative.

Finally, the method can be easily extended to time-periodic Hamiltonians. The simplest case is the hydrogen atom in an oscillatory electric field, a problem widely studied in recent years, both in the optical domain and for a microwave applied to Rydberg states. The Hamiltonian is, in atomic units, and using the length gauge (Casati *et al* 1988, Buchleitner and Delande 1993a):

$$H = \frac{1}{2}p^2 - \frac{1}{r} + Fz \cos \omega t \quad (30)$$

where F and ω denote, respectively, the electric field amplitude and the frequency of the microwave in atomic units of $5.14 \times 10^{11} \text{ V m}^{-1}$ and $4.13 \times 10^{16} \text{ Hz}$. This problem has again the azimuthal symmetry around the field axis and L_z is a good quantum number.

The rotated Hamiltonian is written:

$$H(\theta) = \frac{1}{2}p^2 e^{-2i\theta} - \frac{e^{-i\theta}}{r} + Fz e^{i\theta} \cos \omega t. \quad (31)$$

Although the preceding discussion on the Green function was restricted to a time-independent Hamiltonian, the Floquet theorem allows one to extend the approach to time-periodic systems like equation (30), at the price of adding an additional quantum number corresponding to the number of photons exchanged between the atom and the field. The details can be found in Buchleitner *et al* (1994) and Maquet *et al* (1983). The important point is that only the spatial degrees of freedom need to be made complex: the time itself remains purely real, which preserves the periodicity and permits the use of the Floquet theorem for the complex rotated Hamiltonian. Instead of static eigenstates, one gets time-periodic eigenstates (Brandas and Elander 1989) which can be expanded in their Fourier components:

$$|\psi_{i\theta}(t)\rangle = \sum_K e^{-iK\omega t} |\psi_{i\theta}^K\rangle. \quad (32)$$

The expansion of the $|\psi_{i\theta}^K\rangle$ onto the Sturmian basis, as well as the associated quasi-energies $E_{i\theta}$, can be obtained from a numerical diagonalization of the rotated Floquet Hamiltonian, similarly to the magnetic field case, see Buchleitner *et al* (1994). The electronic densities of the resonances are of course time-dependent. In addition to the exponential decay to the continuum with the rate $-2\text{Im}(E_{i\theta})$, they display the periodicity of the external field. The result is a simple extension of equation (28):

$$|\psi_i(\mathbf{r}, t)|^2 = e^{2\text{Im}E_{i\theta}t} \text{Re} \left\{ \sum_{K, K'} e^{-i(K-K')\omega t} \langle \mathbf{r} | R(-\theta) | \psi_{i\theta}^K \rangle \langle \overline{\psi_{i\theta}^{K'}} | R(\theta) | \mathbf{r} \rangle \right\}. \quad (33)$$

Figure 4 shows the time evolution of the electronic density of a Floquet eigenstate (Rydberg state of principal quantum number $\simeq 23$) over a period of the microwave. This is a relatively narrow isolated resonance, and the electronic density is mainly positive. However, as previously discussed, there are small regions of space where it is negative (magnitude is a few per cent of the maximum). The wavefunction shows a complicated nodal structure which corresponds to the partly chaotic classical behaviour.

The possibility of studying the wavefunctions of resonances has been recently applied (Buchleitner and Delande 1993, Pont *et al* 1993) to the study of the so-called adiabatic

Figure 4. Electronic density of a resonance of the hydrogen atom in a microwave field. It displays an oscillatory time dependence with the period of the driving field. Phase of the microwave field: (a) 0; (b) $\frac{1}{4}\pi$; (c) $\frac{1}{2}\pi$; (d) $\frac{3}{4}\pi$; (e) π . The time evolution is simply inverted for the other half-period. $F = 1.96 \times 10^{-7}$ au; $\omega = 1.07 \times 10^{-4}$ au; $z, \rho = \pm 1300$ au; Complex energy of the resonance: $-9.4836 \times 10^{-4} - i 4.66 \times 10^{-9}$ au.

stabilization (Vos and Gavrila 1992, Potvliege and Smith 1993): when a very strong oscillatory field is applied onto an atom in a weakly excited state, the lifetime of the atomic resonance first decreases with the amplitude of the external field—as expected from a perturbative approach—then reaches a minimum and further *increases* for stronger fields. It has been proposed that this phenomenon is due to a ‘dichotomy’ of the electronic density (Kulander *et al* 1991, Pont *et al* 1990, Su *et al* 1990). In contrast, the numerical study of the electronic density together with the width of the resonance, as done in Buchleitner and Delande (1993b) and Pont *et al* (1993) shows that dichotomy (or polytomy) of the electronic density is *not* a necessary condition for adiabatic stabilization to occur and, hence, *not* at the origin of this interesting phenomenon (see figure 4 in Buchleitner and Delande (1993b)).

The same method can be used for a simplified model, namely a one-dimensional hydrogen atom in a microwave field. The Hamiltonian is obtained from equation (30) simply by forgetting about the degree of freedom along the transverse ρ coordinate. Important results concerning the quantum behaviour of this classically chaotic system have been obtained in the past years (Casati *et al* 1988). However, in practically all these studies, the ionization of the atom is neglected. The method described here allows one to take into account *without any approximation* the effect of the atomic continuum, at the cost of manipulating complex symmetric matrices instead of real ones. An example of a ‘chaotic’ electronic density for a Floquet state, and its evolution over one period of the microwave field, is shown in figure 5. As for the three-dimensional problem, the spectrum and the resonance wavefunctions are generated by numerical diagonalization of

Figure 5. Electronic density of a resonance of a one-dimensional hydrogen atom in a microwave field. This shows that, for an isolated resonance, the electronic density is positive almost everywhere. Phase of the microwave field: (a) 0; (b) $\frac{1}{4}\pi$; (c) $\frac{1}{2}\pi$; (d) $\frac{3}{4}\pi$; (e) π . The time evolution is simply inverted for the other half-period. $F = 2.37 \times 10^{-9}$ au; $\omega = 5.47 \times 10^{-6}$ au. Complex energy of the resonance: $-1.2805 \times 10^{-3} - i 2.1 \times 10^{-11}$ au.

the complex rotated Hamiltonian in a (one-dimensional) Sturmian basis (Buchleitner 1993). The electronic density displays apparently erratic structures, not obviously related to any classical behaviour, with predominant positive values and only tiny negative ones.

In conclusion, the complex coordinate method makes it possible to explore the properties of atomic resonances embedded in a continuum. All the relevant quantities for the physics—position, width, oscillator strength, cross section, electronic density in configuration or phase space...—can be easily and directly obtained by an analytic continuation in the complex energy plane. The various examples presented here show that the method can be used in a practical calculation.

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