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Atoms in circularly polarised fields: the dilatation-analytic approach

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Abstract. The time-evolution operator associated with an atom in a circularly polarised radiation field can be factorised as $U(t) = \exp[-i\omega J_3 t]\exp[-iHt]$, where J_3 is the component of the total angular momentum orthogonal to the two field components and H can explictly be given in terms of the atomic Hamiltonian. We establish, for a one-electron model, the self-adjointness of H and in addition we develop a complex dilatation theory for this operator. The purpose of this approach is to obtain an analytic continuation theory for multiphoton processes so that the imaginary parts of the complex eigenvalues of the complex dilated Hamiltonian $H(\zeta)$ can be related to the various rate constants that govern such processes.

1. Introduction

Consider an atom placed in a monochromatic, spatially homogeneous, circularly polarised external radiation field. It has been known for some time that there exists a time-dependent unitary transformation by means of which the time dependence of the Hamiltonian can be removed (Bunkin and Prokhorov 1964, Salzman 1974). In fact we encounter here an example of a reduction to the Floquet form with an explicitly known Floquet Hamiltonian (for the Floquet approach, see Shirley (1965)). In atomic units the Hamiltonian for the system under consideration is given by

$$H(t) = \sum_{j=0}^{N} (2m_j)^{-1}[\boldsymbol{p}_j - e_j\boldsymbol{A}(t)]^2 + V + W. \tag{1.1}$$

The particle $j = 0$ is the nucleus with mass m_0 and charge $e_0 = N$, whereas the particles $j = 1$ to N are the electrons with charge $e_j = -1$ and mass $m_j = 1$. With particle j are associated its coordinate vector $\boldsymbol{x}_j$, momentum vector $\boldsymbol{p}_j$, orbital angular momentum vector $\boldsymbol{l}_j = \boldsymbol{x}_j \times \boldsymbol{p}_j$ and spin angular momentum vector $\boldsymbol{s}_j$. The total angular momentum is then $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, $\boldsymbol{L} = \Sigma_{j=0}^{N} \boldsymbol{l}_j$, $\boldsymbol{S} = \Sigma_{j=0}^{N} \boldsymbol{s}_j$. In (1.1) coordinates are measured in units a_0 (the Bohr radius), masses in units m (the electronic mass) and charges in units e (the absolute value of the electronic charge). The vector potential $\boldsymbol{A}$ is measured in units $ea_0/\hbar$ ($\boldsymbol{E} = -\partial_t\boldsymbol{A}$, $\boldsymbol{E}$ being the electric field), time in units $ma_0^2/\hbar$ and angular frequency ω in units $\hbar/(ma_0^2)$. The vector potential is given by

$$\boldsymbol{A}(t) = \{A \cos \omega t, A \sin \omega t, 0\}, \tag{1.2}$$

V is the sum of all Coulomb potentials between the particles and W the sum of all their spin–spin and spin–orbit interactions. $H(t)$ is acting in $\mathscr{H} = \mathscr{H}_c \otimes \mathscr{H}_s$, the direct product of the configuration Hilbert space $\mathscr{H}_c = L^2(\mathbb{R}^{3(N+1)}, \mathrm{d}\boldsymbol{x}_0 \ldots \mathrm{d}\boldsymbol{x}_N)$ and the spin Hilbert space $\mathscr{H}_s$. We take for granted that $H(t)$ is self-adjoint with time-independent domain $\mathscr{D}(T) = \mathscr{D}$, $T = \Sigma_{j=0}^N \boldsymbol{p}_j^2/(2m_j)$. (This presupposes that the various terms in W are not too singular in the points $\boldsymbol{x}_i = \boldsymbol{x}_j$.) The equation for the time-evolution operator is

$$\partial_t U(t, t_0) = -\mathrm{i}H(t)U(t, t_0), \qquad U(t_0, t_0) = 1. \tag{1.3}$$

General methods exist (Kato 1953, 1970, Yosida 1966) in order to establish that (1.3) has a unique solution.

We note in passing that an equivalent formulation can be given in terms of

$$H'(t) = T + V + W - \sum_j e_j \boldsymbol{x} \cdot \boldsymbol{E}(t) = H^{\mathrm{at}} - \sum_j e_j \boldsymbol{x} \cdot \boldsymbol{E}(t). \tag{1.4}$$

The corresponding time-evolution operator $\mathscr{W}(t, t_0)$ is related to $U(t, t_0)$ by

$$\mathscr{W}(t, t_0) = X(t)U(t, t_0)X^{-1}(t_0), \qquad X(t) = \exp\Big(\mathrm{i}\sum_j e_j \boldsymbol{x}_j \cdot \boldsymbol{A}(t)\Big). \tag{1.5}$$

We now introduce the group of unitary operators $\{R(t) = \exp(-\mathrm{i}\omega J_3 t), t \in \mathbb{R}\}$. $R(t)$ leaves $\mathscr{D}(T)$ invariant and, since V and W are rotationally invariant,

$$R(t)VR(t)^{-1}f = Vf, \qquad R(t)WR(t)^{-1}f = Wf, \qquad f \in \mathscr{D}. \tag{1.6}$$

The momenta, however, are affected by this transformation. For $f \in \mathscr{D}$ we have $(i = 0, \ldots, N)$

$$\begin{aligned} R(t)p_{i1}R(t)^{-1}f &= (\cos\omega t\, p_{i1} + \sin\omega t\, p_{i2})f, \\ R(t)p_{i2}R(t)^{-1}f &= (-\sin\omega t\, p_{i1} + \cos\omega t\, p_{i2})f, \\ R(t)p_{i3}R(t)^{-1}f &= p_{i3}f, \end{aligned} \tag{1.7}$$

so that, again for $f \in \mathscr{D}$,

$$R(t)[\boldsymbol{p}_j - e_j\boldsymbol{A}(t)]^2 R(t)^{-1}f = (\boldsymbol{p}_j - e_j\boldsymbol{a})^2 f, \tag{1.8}$$

with $\boldsymbol{a} = \{A, 0, 0\}$. Thus

$$\partial_t U(t, t_0) = -\mathrm{i}R(t)\Big(\sum_{j=0}^N (2m_j)^{-1}(\boldsymbol{p}_j - e_j\boldsymbol{a})^2 + V + W\Big)R^{-1}(t)U(t, t_0), \tag{1.9}$$

or

$$\partial_t R^{-1}(t)U(t, t_0)R(t_0) = -\mathrm{i}HR^{-1}(t)U(t, t_0)R(t_0), \tag{1.10}$$

where

$$H = \sum_{j=0}^N (2m_j)^{-1}(\boldsymbol{p}_j - e_j\boldsymbol{a})^2 + V + W - \omega J_3. \tag{1.11}$$

Thus

$$U(t, t_0) = \exp(-\mathrm{i}\omega J_3 t)\exp[-\mathrm{i}H(t - t_0)]\exp(\mathrm{i}\omega J_3 t_0). \tag{1.12}$$

Although the above manipulations have only a formal significance, they can be given an exact meaning provided H, which is a symmetric operator with domain $\mathscr{D}(T) \cap \mathscr{D}(J_3)$, has a unique self-adjoint extension. In the sequel we shall demonstrate this for a special case. Since J_3 is the third component of the total angular momentum, its eigenvalues are either $\pm 1, \pm 2, \ldots$ or $\pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$, depending upon S_3 having integer or half-integer eigenvalues. In the first case $U(t, t_0)$ has the structure predicted by Floquet theory (a Hilbert space version of this theory is discussed in Prugovečki and Tip (1974)), since $\exp(-i\omega J_3 t)$ is periodic with period $2\pi/\omega$. This is also true in the second case if we write

$$U(t, t_0) = \exp[-i\omega(J_3 + \tfrac{1}{2})t] \exp[-i(H - \tfrac{1}{2}\omega)(t - t_0)] \exp[i\omega(J_3 + \tfrac{1}{2})t_0]. \tag{1.13}$$

In the following we shall refer to H as the Floquet Hamiltonian. We note that H is unitarily equivalent to

$$\hat{H} = H^{\mathrm{at}} - \omega J_3 - \omega a \sum_{j=0}^{N} e_j x_{j2}, \tag{1.14}$$

the connecting unitary transformation being generated by $Q = \exp(-i\sum_{j=0}^{N} e_j \boldsymbol{x}_j \boldsymbol{a})$. In the Born–Oppenheimer approximation (fixed nucleus in the origin) and neglecting spin, (1.14) is the Hamiltonian for an atom placed in an electric field with magnitude $E = -\omega a$ in the $\hat{X}_2$ direction and a magnetic field with magnitude $B = -\omega$ in the $\hat{X}_3$ direction but with the diamagnetic contributions to the Hamiltonian omitted.

In practical cases, such as multiphoton ionisation of alkali atoms (e.g. Aymar and Crance 1980) the atomic Hamiltonian is approximated by a spin-independent potential model with a rotationally invariant real potential $V(r)$, $r = |\boldsymbol{x}|$, which takes into account the interaction of the valence electron with the remainder of the atom. In the Born–Oppenheimer approximation the Floquet Hamiltonian then reduces to

$$H = (\boldsymbol{p} - \boldsymbol{a})^2 - \omega l_3 + V(r) = H_0(\boldsymbol{a}) + V(r). \tag{1.15}$$

acting in $\mathscr{H} = L^2(\mathbb{R}^3)$. For hydrogen $V(r) = -r^{-1}$ (note that we made a scale transformation in order to remove the factor $\frac{1}{2}$ in the first term in the middle expression).

In the remaining sections of this paper we study various properties of the Hamiltonian (1.15). This is a non-trivial matter since the presence of the Zeeman term $-\omega l_3$ destroys the semiboundedness of H from below. Nevertheless we shall be able to derive $H_0(\boldsymbol{a})$ compactness of $V(r)$ for a class of potentials including the Coulomb potential. We also expect that there will be a rich resonance structure associated with H. In the hydrogenic case, for instance, $\boldsymbol{p}^2 - \omega l_3 - r^{-1}$ has continuum-embedded eigenvalues $\varepsilon_{nlm} = \varepsilon_n - m\omega$. Although these eigenvalues have associated eigenvectors in symmetry subspaces orthogonal to those associated with the embedding continua, the term $-2\boldsymbol{p}\cdot\boldsymbol{a}$ couples them and this is usually a mechanism that gives rise to resonances. Note that the presence of the Zeeman term prevents one from 'gauging away' the constant vector $\boldsymbol{a}$ in (1.15). In fact one ends up with the corresponding version of (1.14) with the electric field term present. Since the dilation analytic method is a convenient means to study resonances (Combes 1974, Reinhardt 1982, Simon 1973) we shall consider the dilation analytic properties of H. Here we meet a complication since the domain of H changes upon complex dilatation. This rules out a discussion in terms of analytic families of type A or type C (Kato 1966, ch 7), whereas the lack of semiboundedness of the spectrum of H rules out analytic families of type B. We circumvent this problem by first considering the complex dilated Hamiltonian (which has constant domain) and then consider the limit, where the dilatation becomes real.

In § 2 we prove the essential self-adjointness of H, given by (1.15), defined on $\mathscr{S}$ (the functions of rapid decrease) and we show that (1.12) is indeed the solution of

(1.3) for this special case. In §§ 3 and 4 we develop a complex dilatation theory. In § 5 we briefly discuss the connection with multiphoton iniosation processes. A detailed account of the latter, together with applications and numerical results, will be the subject of a forthcoming paper (Muller and Tip 1983). Also in § 5 we discuss the relation between the present work and other recent articles on the subject of atoms in constant and time-dependent fields. For a discussion of the basic mathematical notations occurring in the present work we refer to Kato (1966).

2. Self-adjointness of the Floquet Hamiltonian

In this section we show that $V(r)$ in (1.15) is $H_0(\boldsymbol{a})$ bounded with relative bound smaller than one, respectively $H_0(\boldsymbol{a})$ compact, under essentially the same conditions that it is T bounded ($T=\boldsymbol{p}^2$) with relative bound smaller than one, respectively T compact. We start by noting that

$$H=M\hat{H}M^{-1} \tag{2.1}$$

where $M=\exp(-\mathrm{i}ap_2/\omega)$ and

$$\hat{H}=\boldsymbol{p}^2-\omega l_3+V(\boldsymbol{x}+\boldsymbol{b})+a^2=T-\omega l_3+V(\boldsymbol{x}+\boldsymbol{b})+a^2=H_0+V(\boldsymbol{x}+\boldsymbol{b})+a^2, \tag{2.2}$$

with $\boldsymbol{b}=\{0, a, 0\}$. The unitary equivalence expressed by (2.1) becomes precise once the self-adjointness of $\hat{H}$ has been established. In $H_0=T-\omega l_3$, T and ωl_3 commute (in the sense that $\exp(\mathrm{i}Tt)$ and $\exp(\mathrm{i}\omega l_3 t)$, t real, commute) and each eigenspace $\mathscr{H}_m=P_m\mathscr{H}$ of

$$l_3=\sum_{m=-\infty}^{+\infty} mP_m \tag{2.3}$$

reduces H_0, the reduction of H_0 to $\mathscr{H}_m$ being given by (T_m is the reduction of T to $\mathscr{H}_m$)

$$H_{0m}=T_m-m\omega. \tag{2.4}$$

In the momentum representation T_m is a real multiplication operator and consequently H_{0m} with domain $\mathscr{D}_m=(\mathrm{i}+H_{0m})^{-1}\mathscr{H}_m\subset\mathscr{H}_m$ is self-adjoint on $\mathscr{H}_m$. Let now $\mathscr{D}=\{f=\oplus_m f_m|f_m\in\mathscr{D}_m, \Sigma_m \|H_{0m}f_m\|_m^2<\infty\}$ ($\|\cdot\|_m$ is the norm in $\mathscr{H}_m$) and define $\bar{H}_0 f$ for $f\in\mathscr{D}$ by $\bar{H}_0 f=\oplus_m H_{0m}f_n$. It is straightforward to show that $\bar{H}_0$, thus defined, is self-adjoint. We note that $\mathscr{D}$ contains $\mathscr{D}_0=\mathscr{D}(T)\cap\mathscr{D}(l_3)$. In fact it is strictly larger than $\mathscr{D}_0$, since f, given by $f=\oplus_{m=0}^{\infty} f_m$, $f_m(p)=p^{-1}(1+p^2)^{-1/2}[(p^2-m\omega)^2+1]^{-1/2}h_m$ with $\Sigma_{m=0}^{\infty}|h_m|^2<\infty$ but for which $\Sigma_{m=0}^{\infty} m^{1/2}|h_m|^2$ diverges, is not contained in $\mathscr{D}(T)$ nor in $\mathscr{D}(l_3)$.

Proposition 2.1. $\mathscr{S}$, the Schwartz space of rapidly decreasing functions, is a core of $\bar{H}_0$.

Proof. We note that the notions of closedness and core are invariant under a unitary transformation from one Hilbert space to another. Since $\mathscr{S}$ is invariant under the Fourier transformation and the latter defines the unitary transformation between the coordinate and momentum representation it follows that $\mathscr{S}$ is a core in the coordinate representation if it is one in the momentum representation. We prove the latter. Let $f\in\mathscr{S}$. Then $H_0 f=[\boldsymbol{p}^2+\mathrm{i}\omega(p_1\partial_{p_2}-p_2\partial_{p_1})]f$ is again in $\mathscr{S}$. We denote the restriction of H_0 to $\mathscr{S}$ by $\check{H}_0$. Since $\mathscr{S}\subset\mathscr{D}_0\subset\mathscr{D}$ it follows that $\bar{H}_0\subset\check{H}_0^*$ and $\bar{H}_0=\check{H}_0^{**}\subset\bar{H}_0$. It remains to show that $\check{H}_0^*\subset\bar{H}_0$. Let therefore $g\in\mathscr{D}(\check{H}_0^*)$ and let $\Phi(f)=(f, \check{H}_0^* g)$, so that

$|\Phi(f)| \leq c\|f\|$. Taking $f \in \mathscr{D}$ we have $(\bar{H}_0 f, g) = (f, \check{H}_0^* g) = \Phi(f)$. In particular we have for $f_m \in \mathscr{D}_m \subset \mathscr{D}$ that $|\Phi(f_m)| \leq c\|f_m\|_m$. On the other hand $\Phi(f_m) = (H_{0m} f_m, g_m)_m$, where $g_m = P_m g$. Since the domain of the adjoint A^* of a densely defined operator A in a Hilbert space $\mathscr{H}$ is $\mathscr{D}(A^*) = \{g \in \mathscr{H} |\, |(Af, g)| \leq c\|f\|,\ \forall f \in \mathscr{D}(A)\}$ it follows that $g_m \in \mathscr{D}(H_{0m}^*) = \mathscr{D}(H_{0m}) = \mathscr{D}_m$. Thus $\Phi(f_m) = (f_m, H_{0m} g_m)$ and, with $f^N = \oplus_{m=-N}^N f_m, \Phi(f^N) = \Sigma_{m=-N}^N (f_m, H_{0m} g_m)_m = (f^N, \oplus_{m=-N}^N H_{0m} g_m)$. But $|\Phi(f)| \leq cf$ for every $f \in \oplus_{m=-N}^N \mathscr{H}_m$ so that it follows that $\|\oplus_{m=-N}^N H_{0m} g_m\| \leq c$, i.e. $\Sigma_{m=-N}^N \|H_{0m} g_m\|_m^2 \leq c^2$. Since c does not depend on N it follows that $\Sigma_{M=-\infty}^{+\infty} \|H_{0m} g_m\|_m^2 < \infty$, i.e. $g \in \mathscr{D}$.

In the coordinate representation we have for $f \in \mathscr{S}$

$$(H_0 f)(\boldsymbol{x}) = (-\partial_{\boldsymbol{x}}^2 + \mathrm{i}\omega(x_1 \partial_{x_2} - x_2 \partial_{x_1})] f(\boldsymbol{x}). \tag{2.5}$$

This expression indicates that the difference in the domains of T and H_0 can be traced to the presence of x_1 and x_2 in (2.5). This suggests the use of a cut-off function in coordinate space. We define

$$\Phi(r) = \begin{cases} 1, & 0 \leq r \leq \rho, \\ [1 + (r-\rho)^2]^{-\alpha}, & \alpha \geq 1, r > \rho, \end{cases} \tag{2.6}$$

and we write

$$V(\boldsymbol{x} + \boldsymbol{b}) = V_1(\boldsymbol{x}) + V_2(\boldsymbol{x}) \qquad V_1(\boldsymbol{x}) = V(\boldsymbol{x} + \boldsymbol{b})\Phi(r), \qquad V_2(\boldsymbol{x}) = V(\boldsymbol{x} + \boldsymbol{b})[1 - \Phi(r)]. \tag{2.7}$$

At this point we assume that the real potential $V(r)$ possesses the property:

(A): $V(r)$ is T bounded with T bound smaller than one and $V(r)$ is essentially bounded for $r > r_0 > 0$.

Taking $\rho > r_0 + b$ it follows that $V_2(\boldsymbol{x})$ defines a bounded multiplication operator so that it remains to consider V_1. In the following we denote by $\mathscr{D}$ the domain of $\bar{H}_0$, the closure of H_0, in the coordinate representation (thus its elements are the Fourier transforms of the domain $\mathscr{D}$, introduced earlier).

Lemma 2.1. Let $f \in \mathscr{S}$. Then $\Phi f \in \mathscr{D}(T)$ (the elements of $L^2(\mathbb{R}^2, \mathrm{d}\boldsymbol{x})$ with Fourier transforms $\tilde{f}(\boldsymbol{p})$ with property $p^2 \tilde{f}(\boldsymbol{p}) \in L^2(\mathbb{R}^3, \mathrm{d}\boldsymbol{p})$) and

$$\|T\Phi f\| \leq (1+\varepsilon)\|H_0 f\| + b(\varepsilon)\|f\|, \tag{2.8}$$

with $b(\varepsilon)$ non-negative and where $\varepsilon > 0$ can be chosen arbitrarily small.

The proof of this lemma, which amounts to a repeated use of inequalities, is given in appendix 1.

Lemma 2.2. Let $V(r)$ have property (A). Then V_1 is $\bar{H}_0$ bounded with $\bar{H}_0$ bound smaller than one.

Proof. Let $f \in \mathscr{S}$. Then, denoting the T bound of V by α, $0 < \alpha < 1$,

$$\|V_1 f\| = \|V\Phi f\| \leq \alpha\|T\Phi f\| + \beta\|\Phi f\| \leq \alpha(1+\varepsilon)\|H_0 f\| + \beta\|f\| = \gamma\|H_0 f\| + \beta\|f\|, \tag{2.9}$$

where γ can be made smaller than one by choosing ε sufficiently small. Since $\mathscr{S}$ is a core of $\bar{H}_0$, (2.9) can be extended to $\mathscr{D}$. In case V_1 is not defined for some $f \in \mathscr{D}$ its domain can be extended to $\mathscr{D}$ by a standard limiting procedure: $\mathscr{S}$ being a core of

$\bar{H}_0$, there is a sequence $\{f_n\} \subset \mathcal{S}$ such that $f_n \to f \in \mathcal{D}$ and $H_0 f_n \to \bar{H}_0 f$. Now (2.9) applied to $V_1(f_n - f_m)$ shows that $\{V_1 f_n\}$ is a Cauchy sequence and we define $V_1 f$ by its limit.

Since V_2 is bounded, we have proven:

Theorem 2.1. Let V have property (A). Then $\hat{H} = H_0 + V(\boldsymbol{x} + \boldsymbol{b}) + a^2$ as defined by (2.2) is essentially self-adjoint on $\mathcal{S}$ and the domain of its unique self-adjoint extension $\bar{\hat{H}}$ is $\mathcal{D}$.

Corollary 2.1. $H = (\boldsymbol{p} - \boldsymbol{a})^2 - \omega l_3 + V(r)$, as defined by (1.16), is essentially self-adjoint on $\mathcal{S}$ and the domain of its closure $\bar{H}$ is $M^{-1}\mathcal{D}$.

Proof. A unitary operator U maps a self-adjoint operator A with domain $\mathcal{D}(A)$ into a self-adjoint operator $A' = UAU^{-1}$ with domain $U\mathcal{D}(A)$. In addition it maps a core of A into a core of A'. In our case $U = M$ and M leaves $\mathcal{S}$ invariant.

We now formulate a second condition on $V(r)$:

(B): $V(r)$ is T compact, essentially bounded for $r > r_0 > 0$ and $\lim_{\rho\to\infty} \sup_{r>\rho} |V(r)| = 0$. (Then $V(\boldsymbol{x}+\boldsymbol{b})$ is T compact and $\lim_{\rho\to\infty} \sup_{r>\rho} |V(\boldsymbol{x}+\boldsymbol{b})| = 0$.)
We note that (B) implies (A). A sufficient condition for (B) to be true is that $V(r)$ is locally square integrable and is contained in L^∞ for $r \geq r_0$ with the property $\lim_{\rho\to\infty} \sup_{r>\rho} |V(r)| = 0$ ($V(r) \in L^2 + (L^\infty)_\varepsilon$). As is well known these properties imply that V is T compact.

Theorem 2.2. Let $V(r)$ have property (B). Then $V(\boldsymbol{x} + \boldsymbol{b})$ is $\bar{H}_0$ compact.

Proof. We first show that V_1 is $\bar{H}_0$ compact. Let $z \in \rho(\bar{H}_0)$, the resolvent set of $\bar{H}_0$. Then there is for every $f \in \mathcal{D}$ a unique $g \in \mathcal{H}$ with $f = (z - \bar{H}_0)^{-1} g$. It follows from (2.8) that for $f \in \mathcal{S}$, $f = (z - \bar{H}_0)^{-1} g$

$$\|T\Phi(z - \bar{H}_0)^{-1} g\| \leq (1+\varepsilon)\|\bar{H}_0(z - \bar{H}_0)^{-1} g\| + b(\varepsilon)\|(z - \bar{H}_0)^{-1}\|\|g\| \leq k\|g\|,$$

where k is a positive constant. Since $\mathcal{S}$ is a core of $\bar{H}_0$ it follows that $T\Phi(z - \bar{H}_0)^{-1}$ defines a bounded operator. Now $V_1(\boldsymbol{x})(z - \bar{H}_0)^{-1} = V(\boldsymbol{x} + \boldsymbol{b})(1+T)^{-1} \times (1+T)\Phi(z - \bar{H}_0)^{-1}$ is the product of a compact operator ($V(\boldsymbol{x} + \boldsymbol{b}(1+T)^{-1}$) and a bounded operator $((1+T)\Phi(z - \bar{H}_0)^{-1}$ and hence is compact, i.e. $V_1(\boldsymbol{x})$ is $\bar{H}_0$ compact.

Let $f \in \mathcal{H}$ and $z \in \rho(\bar{H}_0)$. Then

$$\|V(\boldsymbol{x} + \boldsymbol{b})(z - \bar{H}_0)^{-1} f - V_1(z - \bar{H}_0)^{-1} f\| = \|V_2(\boldsymbol{x})(z - \bar{H}_0)^{-1} f\| \leq \|V_2\|_\infty \|(z - \bar{H}_0)^{-1}\| \|f\|. \tag{2.10}$$

But $\|V_2\|_\infty = \sup|V(\boldsymbol{x} + \boldsymbol{b})[1 - \Phi(r)]| \leq \sup_{r>\rho} |V(\boldsymbol{x} + \boldsymbol{b})|$ tends to zero for $\rho \to \infty$, so that it follows from (2.10) that $V(\boldsymbol{x} + \boldsymbol{b})(z - \bar{H}_0)^{-1}$ is the uniform limit of a family of compact operators and hence is itself compact, i.e. $V(\boldsymbol{x} + \boldsymbol{b})$ is $\bar{H}_0$ compact.

Let $H_0(\boldsymbol{a}) = (\boldsymbol{p} - \boldsymbol{a})^2 - \omega l_3$ as in (1.15). It is clear from the above (corollary 2.1 with $V(r) = 0$) that $H_0(\boldsymbol{a})$ is essentially self-adjoint on $\mathcal{S}$ and its closure $\bar{H}_0(\boldsymbol{a})$ has domain $M^{-1}\mathcal{D}$. We can now formulate:

Corollary 2.2. Let $V(r)$ have property (B). Then $V(r)$ is $\bar{H}_0(\boldsymbol{a})$ compact. In particular this is true for the Coulomb potential.

It follows from this result that $\bar{H}$ and $\bar{H}_0(\boldsymbol{a})$ have the same essential spectrum. Since $\bar{H}_0(\boldsymbol{a})-a^2$ and $\bar{H}_0$ are unitarily equivalent and H_{0m}, $m\in\mathbb{Z}$ has spectrum $[-m\omega,\infty)$ it follows that the essential spectrum of $\bar{H}$ covers the real axis. Thus the $\bar{H}_0(\boldsymbol{a})$ compactness of $V(r)$ does not lead to detailed information about the spectrum of H. This becomes quite different upon complex dilatation as will be discussed in the following sections.

We close this section with a demonstration of the fact that $\hat{U}(t)=\exp(-\mathrm{i}\omega l_3 t)\exp(-\mathrm{i}\bar{H}t)$ is the solution of (we put $t_0=0$ in $U(t,t_0)$ and write $U(t)=U(t,0)$)

$$\partial_t U(t)f=-\mathrm{i}H(t)U(t)f, \qquad U(0)=I, \tag{2.11}$$

where

$$H(t)=[\boldsymbol{p}-A(t)]^2+V(r) \tag{2.12}$$

and $f\in\mathscr{D}(H(t))$. It follows from Kato (1953, 1970), (see also Prugovečki and Tip 1974) that (2.11) has a unique solution $U(t)$. Amongst others, $U(t)$ has the following properties: $U(t)$, $t\in\mathbb{R}$ is strongly continuous in t, it is unitary, $U(t)\mathscr{D}(H(t))\subset\mathscr{D}(H(t))$ (note that $\mathscr{D}(H(t))=\mathscr{D}(T)$) and

$$\partial_t U^*(t)f=\mathrm{i}U^*(t)H(t)f, \qquad f\in\mathscr{D}(T). \tag{2.13}$$

An attempt to show that $\hat{U}(t)=U(t)$ by direct differentiation fails, since, formally,

$$\partial_t\hat{U}(t)f=-\mathrm{i}\exp(\mathrm{i}\omega l_3 t)(\bar{H}+\omega l_3)\exp(-\mathrm{i}\bar{H}t)f$$

and we do not know if $\exp(-\mathrm{i}\bar{H}t)f\in\mathscr{D}_0$ for $f\in\mathscr{D}_0$ (this is the case if $V(r)$ vanishes, as shown in appendix 2). We therefore proceed differently. We note that (2.13) has at least one solution (namely $U^*(t)$) which is unitary and strongly continuous in t.

Let now $W(t)$ be a second solution with these properties. Then, for $f\in\mathscr{D}(T)$ (so that $U(t)f\in\mathscr{D}(T)$)

$$\partial_t W(t)U(t)f=\mathrm{i}W(t)G(t)f+W(T)\cdot -\mathrm{i}H(t)U(t)f=0.$$

Since $W(0)U(0)f=f$, $W(t)U(t)f$ is continuous in t and $W(t)U(t)$ is bounded, it follows that $W(t)U(t)=I$, so that

$$W(t)=W(t)U(t)U^*(t)=IU^*(t)=U^*(t).$$

Let now $f\in\mathscr{D}_0$. Then $\exp[\mathrm{i}\omega l_3 t]f\in\mathscr{D}_0$ and

$$\begin{aligned}\partial_t\hat{U}^*(t)f&=\mathrm{i}\exp(\mathrm{i}\bar{H}t)(\bar{H}+\omega l_3)\exp(\mathrm{i}\omega l_3 t)f\\ &=\mathrm{i}\hat{U}(t)\exp(-\mathrm{i}\omega l_3 t)[(\boldsymbol{p}-\boldsymbol{a})^2+V(r)]\exp(\mathrm{i}\omega l_3 t)f\\ &=\mathrm{i}\hat{U}^*(t)H(t)f,\end{aligned} \tag{2.14}$$

so that

$$U^*(t)f-f=\mathrm{i}\int_0^t \mathrm{d}s\,\hat{U}^*(s)H(s)f=\mathrm{i}\int_0^t \mathrm{d}s\,U^*(s)H(s)(1+T)^{-1}(1+T)f. \tag{2.15}$$

Since $\mathscr{D}_0$ is a core of T there is a sequence $\{g_n\}\subset\mathscr{D}_0$ such that $g_n\to g$ and $Tg_n\to Tg$, $g\in\mathscr{D}(T)$. But then the right-hand side of (2.15) with f replaced by $g-g_n$ tends to zero (since $\int_0^t \mathrm{d}s\,\|H(s)(1+T)^{-1}\|$ is bounded). Thus (2.15) and, by differentiation, (2.14) holds for every $f\in\mathscr{D}(T)$. Since $\hat{U}(t)$ is unitary and strongly continuous we have proven:

Theorem 2.3. $\hat{U}(t)$ is the (unique) solution of (2.11).

3. Complex dilatation of the free Floquet Hamiltonian

We recall that elements of the dilatation group $\{U(\theta)=\exp(\mathrm{i}\theta A),\ \theta\in\mathbb{R},\ A=\frac{1}{2}(\boldsymbol{p}\cdot\boldsymbol{x}+\boldsymbol{x}\cdot\boldsymbol{p})\}$ act on $f(\boldsymbol{x})\in\mathscr{H}$ according to

$$(U(\theta)f)(\boldsymbol{x})=\exp(3\theta/2)f[\exp(\theta)\boldsymbol{x}],$$

whereas in the momentum representation

$$(U(\theta)f)(\boldsymbol{p})=\exp(-3\theta/2)f[\exp(-\theta)\boldsymbol{p}].$$

The operators $\boldsymbol{x}$ and $\boldsymbol{p}$ transform according to

$$U(\theta)\boldsymbol{x}U(\theta)^{-1}=\boldsymbol{x}\exp(\theta)\ \text{and}\ U(\theta)\boldsymbol{p}U(\theta)^{-1}=\boldsymbol{p}\exp(-\theta),$$

whereas the angular momentum $\boldsymbol{l}=\boldsymbol{x}\times\boldsymbol{p}$ is left invariant. Complex dilatation theory is concerned with the analytic continuation of real dilatations (i.e. $\theta\to\zeta\in\mathbb{C}$). Under such transformations the spectral properties of the Hamiltonian sometimes change in a way that makes it possible to treat resonances in terms of complex isolated eigenvalues of the (non-self-adjoint) complex dilated Hamiltonian (Aguilar and Combes 1971, Simon 1973). For the model considered here, we expect the imaginary parts of such eigenvalues to be associated with the various ionisation probabilities occurring in a multiphoton ionisation process. There are two possibilities to implement this program in our case. The first one is to start from the Hamiltonian (1.15), which, upon a real dilatation, takes the form

$$\begin{aligned}H(\theta)&=[\boldsymbol{p}\exp(-\theta)-\boldsymbol{a}]^2-\omega l_3+V[r\exp(+\theta)]=H_0(\boldsymbol{a},\theta)+V[r\exp(+\theta)]\\&=T(\theta)-\omega l_3-2\boldsymbol{a}\cdot\boldsymbol{p}\exp(-\theta)+a^2+V[r\exp(+\theta)]\\&=H_0(\theta)-2\boldsymbol{a}\cdot\boldsymbol{p}\exp(-\theta)+a^2+V[r\exp+\theta)].\end{aligned}\qquad(3.1)$$

The second one is to start from $\hat{H}$, given by (2.2). After a real dilatation this Hamiltonian transforms into

$$\hat{H}(\theta)=H_0(\theta)+a^2+V[\boldsymbol{x}\exp(+\theta)+\boldsymbol{b}].\qquad(3.2)$$

Here we have the attractive feature that $H_0(\theta)$ has simple spectral properties (since T and l_3 commute) but also the drawback that $V(\boldsymbol{x}+\boldsymbol{b})$ is not dilatation analytic, even if $V(r)$ is. This difficulty can be overcome by means of a so-called exterior scaling technique (Simon 1979) but then the simplicity of the standard dilatation transformation is lost. We therefore return to the first alternative (3.1), where we encounter the complication of the symmetry breaking term $-2\boldsymbol{a}\cdot\boldsymbol{p}\exp(-\theta)$. In analysing the spectral properties of the corresponding complex dilated free (i.e. without V) Hamiltonian

$$H_0(\boldsymbol{a},\zeta)=T\exp(-2\zeta)-\omega l_3+a^2-2\boldsymbol{a}\cdot\boldsymbol{p}\exp(-\zeta)=H_0(\zeta)+a^2-2\boldsymbol{a}\cdot\boldsymbol{p}\exp(-\zeta),\qquad(3.3)$$

we find, somewhat surprisingly, that the term $-2\boldsymbol{p}\cdot\boldsymbol{a}\exp(-\zeta)$ does not affect the spectrum of $H_0(\zeta)$. In this respect it acts as if it were a relatively compact perturbation of $H_0(\theta)$. This is not the case but in the momentum representation $H_0(\zeta)$ acts as a multiplication operator in p and ξ (p, ξ and ϕ are the spherical coordinates associated with $\boldsymbol{p}$) and we can make a direct integral decomposition

$$H_0(\zeta) = \int_{\oplus} \mathrm{d}p \, \mathrm{d}\xi \, H_0(\zeta, p, \xi) \tag{3.4}$$

where now on each fibre

$$[-2\boldsymbol{p} \cdot \boldsymbol{a} \exp(-\zeta)](p, \xi) = -2pa \exp(-\zeta) \sin \xi \cos \phi$$

is $H_0(\zeta, 0, \xi)$ compact. We shall, however, follow a different approach. In fact the presence of the Zeeman term $-\omega l_3$ is of paramount importance; if it is deleted $H_0(\boldsymbol{a}, \zeta)$ changes into $[\boldsymbol{p} \exp(-\zeta) - \boldsymbol{a}]^2$, which operator has a totally different spectrum for non-real ζ (a parabola and its inside, see Combes and Thomas (1973)). A further complicating factor is that, although the domain of the complex dilated Hamiltonian does not depend on ζ, it differs from the domain for real $\zeta = \theta$. (Note that both (3.1) and (3.2) have θ-dependent domains.) We overcome this problem by first considering non-real ζ, where we are dealing with an analytic family of type A, and then we show that the generalised strong limit $\operatorname{Im} \zeta \to 0$ exists.

We now introduce some notation. If ζ is complex we often split it according to $\zeta = \theta + \mathrm{i}\psi$, θ, ψ real and we define two open strips in $\mathbb{C}$:

$$I_{\pm} = \{\zeta \in \mathbb{C} | 0 < \pm\psi < \pm\pi/2\}.$$

Further, let $\mathscr{D}_0 = \mathscr{D}(T) \cap \mathscr{D}(l_3) = \mathscr{D}(\boldsymbol{p}^2) \cap \mathscr{D}(l_3)$ as before.

Proposition 3.1. $H_0(\boldsymbol{a}, \zeta) = [\boldsymbol{p} \exp(-\zeta) - \boldsymbol{a}]^2 - \omega l_3$, $\zeta \in I_{\pm}$ with domain $\mathscr{D}_0$ is closed.

Proof. Since $\boldsymbol{p} \cdot \boldsymbol{a}$ is T bounded with arbitrarily small T bound and since $\mathscr{D}_0 \subset \mathscr{D}(T)$ it is sufficient to give the proof for $H_0(\zeta)$. We work in the momentum representation.

The subspaces $\mathscr{H}_m$, introduced in § 2, reduce $H_0(\zeta)$ and

$$H_{0m}(\zeta) = T_m(\zeta) - m\omega = T_m \exp(-2\zeta) - m\omega$$

is closed with domain $\mathscr{D}_m = \mathscr{D}(T_m)$. Now let

$$\mathscr{D}(\zeta) = \left\{ f = \bigoplus_m f_m | f_m \in \mathscr{D}_m, \sum_m \|H_{0m}(\zeta) f_m\|_m^2 < \infty \right\}.$$

For $f \in \mathscr{D}(\zeta)$ we define $H_0(\zeta) f = \oplus_m H_{0m}(\zeta) f_m$. Then $\bar{H}_0(\zeta)$ with domain $\mathscr{D}(\zeta)$ is closed. We show now that $\mathscr{D}(\zeta) = \mathscr{D}_0$, for which it is sufficient to prove that $\mathscr{D}(\zeta) \subset \mathscr{D}_0$. We note that $|\bar{H}_0(\zeta)| = [\bar{H}_0(\zeta)^* \bar{H}_0(\zeta)]^{1/2}$ with domain $\mathscr{D}(\zeta)$ is closed (Kato 1966, p 334). For every $f \in \mathscr{D}(\zeta)$ there is a unique $g \in \mathscr{H}$ with $f = [1 + |\bar{H}_0(\zeta)|]^{-1} g$. Each $\mathscr{H}_m$ reduces $|\bar{H}_0(\zeta)|$ and its restriction to $\mathscr{H}_m$ is given by

$$\begin{aligned} |\bar{H}_0(\zeta)|_m &= [H_{0m}(\zeta)^* H_{0m}(\zeta)]^{1/2} = [T_m^2(\theta) - 2m\omega \cos 2\psi \, T_m(\theta) + m^2\omega^2]^{1/2} \\ &= \{[T_m(\theta) - m\omega \cos 2\psi]^2 + m^2\omega^2 \sin^2 2\psi\}^{1/2} \\ &= [T_m^2(\theta) \sin^2 2\psi + (T_m(\theta) \cos 2\psi - m\omega)^2]^{1/2}. \end{aligned}$$

Now

$$\|l_3 f\|^2 = \sum_m \|m[1 + |\bar{H}_0(\zeta)|_m]^{-1} g_m\|_m^2 \leq \sum_m (\omega \sin 2\psi)^{-2} \|g_m\|_m^2 = (\omega \sin \phi)^{-2} \|g\|^2$$

and

$$\|Tf\|^2 = \sum_m \|T_m[1+|\bar{H}_0(\zeta)|_m]^{-1} g_m\|_m^2 \leq \sum_m (\sin 2\psi \exp -2\theta)^{-2}\|g_m\|_m^2$$

$$= [\sin 2\psi \exp(-2\theta)]^{-2}\|g\|^2$$

so that $f \in \mathscr{D}(l_3)$ and $f \in \mathscr{D}(T)$, i.e. $f \in \mathscr{D}_0$.

Since $\mathscr{D}(T(\zeta)) = \mathscr{D}(T)$ and $\mathscr{D}(l_3(\zeta)) = \mathscr{D}(l_3)$ it follows that $U(\zeta)\mathscr{D}_0 = \mathscr{D}_0$, $\forall \zeta \in \mathbb{C}$. A real dilatation transformation transforms $H_0(\boldsymbol{a}, \zeta)$, $\zeta \in I_\pm$ into $U(\theta_0)H_0(\boldsymbol{a}, \zeta)U(\theta_0)^{-1} = H_0(\boldsymbol{a}, \zeta+\theta_0)$ so that going from $H_0(\boldsymbol{a}, \zeta_0)$ to $H_0(\boldsymbol{a}, \zeta)$, $\zeta_0, \zeta \in I_+(I_-)$ can be interpreted as a complex dilatation transformation. In addition we have:

Proposition 3.2. $\{H_0(\boldsymbol{a}, \zeta), \zeta \in I_\pm\}$ are holomorphic families of type A (for this notion, see Kato 1966, p 375).

Proof. $\mathscr{D}(H_0(\boldsymbol{a}, \zeta)) = \mathscr{D}_0$, independent of $\zeta \in I_+(I_-)$ whereas for each $f \in \mathscr{D}_0$, $H_0(\boldsymbol{a}, \zeta)f$ is a vector-valued analytic function of $\zeta \in I_+(I_-)$.

Proposition 3.3. $K_\pm(\zeta) = \mp \mathrm{i}H_0(\boldsymbol{a}, \zeta) \mp \frac{1}{2}a^2 \tan\psi$, $\zeta \in I_\pm$ generate strongly continuous contraction semigroups.

Proof. We consider $K_+(\zeta)$. We note that

$$K_+(\zeta)^* = \mathrm{i}H_0(\boldsymbol{a}, \bar{\zeta}) - \tfrac{1}{2}a^2 \tan\psi = K_-(\bar{\zeta})$$

and that $K_+(\zeta)$ and $K_+(\zeta)^*$ with domain $\mathscr{D}_0$ are closed. A small computation results in

$$\mathrm{Re}\,(K_+(\zeta)f, f) = \mathrm{Re}\,(K_+^*(\zeta)f, f) = -\sin 2\psi([\boldsymbol{p}\exp(-\theta) - \boldsymbol{a}/(2\cos\psi)]^2 f, f) \leq 0$$

for $\zeta \in I_+$ and for each $f \in \mathscr{D}_0$. Thus $K_+(\zeta)$ and $K_+(\zeta)^*$ are closed dissipative operators and consequently they are generators of strongly continuous contraction semigroups (Lumer and Phillips 1961, p 687).

Remark. Proposition 3.3 also follows from the explicit representation for the associated semigroup as given in appendix 2. The open right half-plane is in the resolvent set of the generator A of a strongly continuous contraction semigroup and $\|(z-A)^{-1}\| \leq (\mathrm{Re}\, z)^{-1}$, $\mathrm{Re}\, z > 0$. Thus:

Corollary 3.1. The resolvent sets $\rho(H_0(\boldsymbol{a}, \zeta))$ of $H_0(\boldsymbol{a}, \zeta)$, $\zeta \in I_\pm$, are not empty. In fact every $z \in \mathbb{C}$ with $\mathrm{Im}\, z > \frac{1}{2}a^2 \tan\psi$ is contained in $\rho(H_0(\boldsymbol{a}, \zeta))$, $\zeta \in I_+$, and

$$\|[z - H_0(\boldsymbol{a}, \zeta)]^{-1}\| \leq (\mathrm{Im}\, z - \tfrac{1}{2}a^2 \tan\psi)^{-1}$$

for such z. Similarly each z with $\mathrm{Im}\, z < \frac{1}{2}a^2 \tan\psi$ is in $\rho(H_0(\boldsymbol{a}, \zeta)) \cdot \zeta \in I_-$, in which case

$$\|[z - H_0(\boldsymbol{a}, \zeta)]^{-1}\| \leq (-\mathrm{Im}\, z + \tfrac{1}{2}a^2 \tan\psi)^{-1}.$$

It follows that for $\zeta \in I_+$ and $\mathrm{Im}\, z > \frac{1}{2}a^2 \tan\psi$

$$[z - H_0(\boldsymbol{a}, \zeta)]^{-1} = -\mathrm{i}\int_0^\infty \mathrm{d}t\, \exp\{\mathrm{i}[z - H_0(\boldsymbol{a}, \zeta)]t\}, \tag{3.5}$$

and a similar expression can be given for $\zeta \in I_-$ and $\operatorname{Im} z < \frac{1}{2}a^2 \tan \psi$. In appendix 2 we prove, starting from (3.5), that for $\zeta \in I_\pm$, $\sigma(H_0(\boldsymbol{a}, \zeta))$, the spectrum of $H_0(\boldsymbol{a}, \zeta)$, is given by the set of half lines

$$\Sigma = \Sigma(a, \zeta) = \Sigma(a, \psi) = \{z = a^2 + \lambda \exp(-2i\psi) + k\omega, \lambda \in [0, \infty], k \in \mathbb{Z}\}. \tag{3.6}$$

We finally note that $[z - H_0(\boldsymbol{a}, \zeta)]^{-1}$ is a bounded, operator-valued analytic function of both z and ζ for $\{z, \zeta\} \in \mathcal{N} = \{\{z, \zeta\} | \zeta \in I_+,\ z \in \rho(H_0(\boldsymbol{a}, \zeta))\}$ (Kato 1966, p 367, theorem 1.3, Reed and Simon 1978, p 14, theorem 12.7).

4. The dilated full Floquet Hamiltonian

Suppose that $V(r)$ is $\bar{H}_0(\boldsymbol{a})$ compact as discussed in § 2. Then $V(\theta) = V[r \exp(\theta)]$ is $\bar{H}_0(\boldsymbol{a}, \theta)$ compact so that $K(z, \theta) = V(\theta)[z - \bar{H}_0(\boldsymbol{a}, \theta)]^{-1}$ is compact for each $\theta \in \mathbb{R}$ and each non-real z. In the usual complex dilatation theory (Aguilar and Combes 1971) an analytic continuation $K(z, \zeta)$ of $K(z, \theta)$ for complex ζ is made. Here we have to proceed in a different way since $\bar{H}_0(\boldsymbol{a}, \zeta)$ does not have a strip containing the real axis in its analyticity domain, due to the fact that $\mathcal{D}(\bar{H}_0(\boldsymbol{a}, \zeta))$ is different for real and complex ζ. We therefore start from $\zeta \in I_+$ and consider the limit $\psi \downarrow 0$. Of course we can also start from $\zeta \in I_-$ and have $\psi \uparrow 0$. We shall not discuss the latter case any further since all statements and proofs are the mirror images of the former ones.

Suppose that $V(r)$ is a dilatation analytic potential with respect to T (in short, T-dilation analytic or T analytic), i.e. $V(\theta)$ has a T compact analytic continuation $V(\zeta)$ for $\zeta \in I_\alpha = \{\zeta \in \mathbb{C} | |\operatorname{Im} \zeta| < \alpha\}$ for some $\alpha > 0$. Then for $z \in \rho(H_0(\boldsymbol{a}, \zeta))$, $\forall \zeta \in I_\beta$, $\beta < \pi/2$,

$$K(z, \zeta) = V(\zeta)[z - H_0(\boldsymbol{a}, \zeta)]^{-1} = V(\zeta)(1 + T)^{-1}(1 + T)[z - H_0(\boldsymbol{a}, \zeta)]^{-1} \tag{4.1}$$

is a compact-operator-valued analytic function of

$$\zeta \in I_\alpha \cap I_+ = I_{\alpha+}.$$

This follows from the fact that, since $\mathcal{D}_0 \subset \mathcal{D}(T)$, $(1 + T)[z - H_0(\boldsymbol{a}, \zeta)]^{-1}$ is bounded analytic and that $V(\zeta)(1 + T)^{-1}$ is compact analytic. Thus $V(\zeta)$ is $H_0(\boldsymbol{a}, \zeta)$compact for $\zeta \in I_{\alpha+}$ so that

$$H(\zeta) = H_0(\boldsymbol{a}, \zeta) + V(\zeta) \tag{4.2}$$

with domain $\mathcal{D}_0$ is closed.

We now assume that $V(r)$ has the following properties:

(C): $V(r)$ has the properties (B), $V(r)$ is T analytic with analyticity domain I_α, $\alpha > 0$ and for

$$V(\zeta) = V(\zeta)\Phi(r) + V(\zeta)[1 - \Phi(r)] = V_1(\zeta) + V_2(\zeta), \tag{4.3}$$

with $\Phi(r)$ given by (2.6), there is a $\rho_0 > 0$, a constant k and a strip $I_0 = \{\zeta | |\operatorname{Im} \zeta| < \psi_0\}$ such that for $\rho > \rho_0$ and $\zeta \in I_0$, $\|V_2(\zeta)\|_\infty \leq k$. (For the Coulomb potential we obviously have no restrictions on ψ.)

If $\|K(z, \zeta)\| \leq \beta < 1$ for some z and ζ then

$$[z - \bar{H}(\zeta)]^{-1} = [z - \bar{H}_0(\boldsymbol{a}, \zeta)]^{-1}[1 - K(z, \zeta)]^{-1}, \tag{4.4}$$

which expression is a convenient starting point for a discussion of the spectral properties of $\bar{H}(\zeta)$ and the limit $\psi \downarrow 0$. (The closure bar is needed since we allow $\psi = 0$. From now on we shall omit the bar when no confusion can arise.) The usual approach to arrive at (4.4) is to make z large negative for Hamiltonians bounded from below. This is obviously not possible here but instead we can make $y = \operatorname{Im} z$ large positive.

Lemma 4.1. Let $V(r)$ have the properties (C). There is a region $\mathcal{M}$ in the open upper half-plane, a strip $I_1 = \{\zeta | 0 \leq \operatorname{Im} \zeta < \psi_1\}$ and a constant $\beta \in (0, 1)$ such that $\|K(z, \zeta)\| \leq \beta$ for every $z \in \mathcal{M}$ and $\zeta \in I_1$.

Proof. Since operator norms and spectra are invariant under real dilatations (which are unitary transformations) we can put $\theta = 0$. Now

$$\|K(z, \mathrm{i}\psi)\| \leq \|V(\mathrm{i}\psi)\Phi[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| + \|V(\mathrm{i}\psi)(1-\Phi)[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\|. \tag{4.5}$$

For ρ sufficiently large we have for $\psi \in [0, \psi_2]$, $\psi_2 = \min\{\psi_0, \pi/4\}$, $\|V(\mathrm{i}\psi)(1-\Phi)\times [z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| \leq k\|[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| \leq k[y - \frac{1}{2}a^2 \tan\psi]^{-1} \leq k(y - \frac{1}{2}a^2)^{-1} < \frac{1}{4}$ for $y > y_1 > 0$ with suitably chosen $y_1 = y_1(k)$.

In Appendix 1 we show that for $f \in \mathcal{S}$

$$\|T\Phi\| \leq k_1\|H_0(\boldsymbol{a}, \mathrm{i}\psi)f\| + k_2\|f\|, \tag{4.6}$$

where k_1 and k_2 are positive constants, independent of $\psi \in [0, \psi_3]$, $\psi_3 \in (0, \pi/4)$. Since $\mathcal{S}$ is a core of $H_0(\boldsymbol{a}, \mathrm{i}\psi)$ (the proof for $\psi \neq 0$ is similar to the one for $\psi = 0$) it follows that (4.6) is true for every $f \in \mathcal{D}(\bar{H}_0(\boldsymbol{a}, \mathrm{i}\psi))$ so that ($y = \operatorname{Im} z > \frac{1}{2}a^2$)

$$\begin{aligned}
&\|(y + T)\Phi[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| \\
&\quad \leq y\|[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| + k_1\|H_0(\boldsymbol{a}, \mathrm{i}\psi)[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| \\
&\qquad + k_2\|[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| \\
&\quad \leq k + (y + k_1|z| + k_2)\|[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| \\
&\quad \leq k_1 + (y + k_1|z| + k_2)(y - \tfrac{1}{2}a^2)^{-1}.
\end{aligned} \tag{4.7}$$

Now there is a curve $y = \mu + \nu|x|$, μ, $\nu > 0$, such that the right-hand side of (4.7) is smaller than a positive constant k_3 for $z = x + \mathrm{i}y$ in the open set $\mathcal{M} \in \mathbb{C}$, consisting of the points above this curve. Thus

$$\begin{aligned}
&\|V(\mathrm{i}\psi)\Phi[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| \\
&\quad = \|V(\mathrm{i}\psi)(y + T)^{-1}(y + T)\Phi[z - H_0(\boldsymbol{a}, \mathrm{i}\psi)]^{-1}\| \leq k_4\|V(\mathrm{i}\psi)(y + T)^{-1}\|.
\end{aligned} \tag{4.8}$$

Since $V = V(0)$ is T compact, there is a $y_2 > 0$, such that $\|V(0)(y + T)^{-1}\| < (8k_3)^{-1}$ for $y > y_2$. Also, $V(\zeta)$ being T analytic, there is a $\psi_4 > 0$, such that for $\psi \in [0, \psi_4]$,

$$\|[V(\mathrm{i}\psi) - V(0)](1 + T)^{-1}\| < (8k_3)^{-1}.$$

Thus for $\psi \in [0, \psi_4]$ and $y > \max\{1, y_2\}$

$$\begin{aligned}
&\|V(\mathrm{i}\psi)(y + T)^{-1}\| \\
&\quad \leq \|V(0)(y + T)^{-1}\| + \|[V(\mathrm{i}\psi) - V(0)](1 + T)^{-1}\| \cdot \|(1 + T)(y + T)^{-1}\| \\
&\quad \leq (4k_4)^{-1}.
\end{aligned} \tag{4.9}$$

Replacing μ above by $\max\{\mu, y_1, y_2, 1\}$ we have $\|K(z, \rho)\| \leq \frac{1}{2}$ for z in the set $\mathcal{M}$ thus defined and for

$$\zeta \in I_1 = \{\zeta | 0 \leq \operatorname{Im} \zeta < \min(\psi_2, \psi_3, \psi_4)\}.$$

Corollary 4.1. There is a constant $k'>0$ such that $\|[z-H(\zeta)]^{-1}\|<k'$ for $z\in\mathcal{M}$ and $\zeta\in I_1$. In addition $[z-H(\zeta)]^{-1}$ is analytic in both z and ζ for $\{z,\zeta\}\in\mathcal{M}+I_2\subset\mathbb{C}\times\mathbb{C}$ where I_2 is in the intersection of $I_{\alpha+}$ and I_1.

Proof. As is clear from the first part of the proof of lemma 4.1, $\|[z-H_0(\boldsymbol{a},\zeta)]^{-1}\|$ is bounded by a constant k'' for $z\in\mathcal{M}$ and $\zeta\in I_1$. Thus, for such z and ζ

$$\|[z-H(\zeta)^{-1}\|\leq k''[1-\|K(z,\zeta)\|]^{-1}\leq 2k''=k'. \tag{4.10}$$

The analyticity follows from the analyticity of $[z-H_0(\boldsymbol{a},\zeta)]^{-1}$ for $\{z,\zeta\}\in\mathcal{N}$ (see § 3), the analyticity of $K(z,\zeta)$ for $\{z,\zeta\}\in\mathcal{N}\cap\mathcal{M}\times I_2$ and the boundedness of $K(z,\zeta)$; $\|K(z,\zeta)\|\leq\frac{1}{2}$.

Theorem 4.1. $H(\theta)$ is the generalised strong limit of $H(\zeta)$ for $\psi\downarrow 0$. In particular

$$\underset{\psi\downarrow 0}{\text{s-lim}}\,[z-H(\zeta)]^{-1}=[z-H(\theta)]^{-1}, \qquad \forall z\in\mathcal{M}. \tag{4.11}$$

Proof. Referring to Kato (1966, p 429, theroem 1.5) and noting that $\mathcal{D}_0$ is a core of $H(\theta)$ (since $\mathcal{S}$ is a core and $\mathcal{S}\subset\mathcal{D}_0$) we have to show two things. The first is that the intersection of $\rho(H(\theta))$ and the region of boundedness of the family $\{H(\zeta),\zeta\in I_{\alpha+}\}$ is not empty. This is clear from the self-adjointness of $H(\theta)$ and the above corollary. The second is that for each $f\in\mathcal{D}_0$, $H(\zeta)f\to H(\theta)f$. Indeed, for $f\in\mathcal{D}_0$

$$\begin{aligned}\|H(\zeta)f-H(\theta)f\|&\\ &\leq|\exp(-2\zeta)-\exp(-2\theta)|\,\|Tf\|+2|\exp(-\zeta)-\exp(-\theta)|\,\|\boldsymbol{p}\cdot\boldsymbol{a}f\|\\ &\quad+\|[V(\zeta)-V(\theta)](1+T)^{-1}\|\,\|(1+T)f\|\end{aligned} \tag{4.12}$$

where all terms on the right tend to zero (the last one since $V(\zeta)$ is T analytic).

We are now in a position to discuss the meromorphic continuation of certain inner products $([z-H(\theta)]^{-1}f,g)=(R(z,\theta)f,g)$. Since physical quantities pertaining to multiphoton ionisation processes can be expressed in terms of such inner products this is a result with important practical consequences. Here we have to deviate in our discussion from the approach followed by Aguilar and Combes since now the real axis is not in the analyticity domain of ζ. Let f and g be analytic vectors for the dilatation group. Then $f(\zeta)=U(\zeta)f$ and $g(\zeta)=U(\zeta)g$ are analytic and their limits for $\psi\downarrow 0$ exist. (In fact we only need meromorphy and the existence of the limits.) Let now

$$F(z,\zeta)=(R(z,\zeta)f(\zeta),g(\zeta)), \qquad \{z,\zeta\}\in\mathcal{M}\times I_2. \tag{4.13}$$

$F(z,\zeta)$ is analytic in $\zeta\in I_2$ and invariant under real dilatations so that it must be ζ independent. According to theorem 4.1, $F(z)=F(z,\theta)=\lim F(z,\zeta)$ for $\psi\downarrow 0$ so that $F(z)=F(z,\zeta)$, $z\in\mathcal{M}$. Since $F(z)$ contains the resolvent of a self-adjoint operator it is analytic in the open upper half-plane. Thus $F(z,\zeta)$, $\zeta\in I_2$, can be analytically continued in the whole open upper half-plane. Next, since $K(z,\zeta)$ is compact analytic in $\{z,\zeta\}\in\mathcal{M}\times I_2$ it follows (Dunford and Schwartz 1959, lemma VII-6.13, Steinberg 1968) that for fixed $\zeta\in I_2$ $[1-K(z,\zeta)]^{-1}$ has a meromorphic extension to all z for which $K(z,\zeta)$ is analytic in z, in particular to all $z\in\rho(H_0(\boldsymbol{a},\zeta))$. Consequently $R(z,\zeta)=R_0(z,\zeta)[1-K(z,\zeta)]^{-1}$, $R_0(z,\zeta)=[z-H_0(\boldsymbol{a},\zeta)]^{-1}$, has such a meromorphic extension and the same is true for $F(z,\zeta)$ (as we have seen $F(z,\zeta)$ is actually analytic in z for z in the open upper half-plane). The various half-lines from Σ are branch cuts for $F(z,\zeta)$, the various 'threshold' $a^2+k\omega$, $k\in\mathbb{Z}$ are branch points. Keeping $z\in\mathcal{M}$ fixed we can continue $[1-K(z,\zeta)]^{-1}$ and $R(z,\zeta)$ meromorphically to all $\zeta\in I_{\alpha+}$ (since $R_0(z,\zeta)$ is bounded analytic and $K(z,\zeta)$ compact analytic for all $\zeta\in I_{\alpha+}$ and fixed $z\in\mathcal{M}$). Thus $F(z,\zeta)$ is meromorphic for $\zeta\in I_{\alpha+}$ and fixed $z\in\mathcal{M}$. But since it is the meromorphic extension of a ζ-independent function it is itself ζ independent and $F(z,\zeta)=F(z)$ as long as the half-lines from Σ are avoided. Since the latter depend on ψ we can control the area into which we can continue a particular branch of $F(z,\zeta)$ by the choice of ψ (see figure 1). $F(z,\zeta)$, as a function of z, can have poles on the real axis and in the lower half-plane outside Σ. These poles are eigenvalues of the dilated Hamiltonian. They have finite multiplicity, are ζ independent but can be uncovered and covered as ψ changes, so that one of the half-lines sweeps over them. Their only accumulation points are the various branch points $a^2+k\omega$, $k\in\mathbb{Z}$ and they do not occur in the open upper half-plane. These results follow in essentially the same way as in Aguilar and Combes (1971). In the present case we do not expect that these eigenvalues are confined to a bounded region in $\mathbb{C}$, due to the presence of the Zeeman term $-\omega l_3$. We also expect that $H(\zeta)$ does not have real eigenvalues but that all eigenvalues have turned into resonances (the poles in the lower half-plane). The physical reason behind this is that an atom always photo-ionises upon absorbing a sufficient amount of photons.

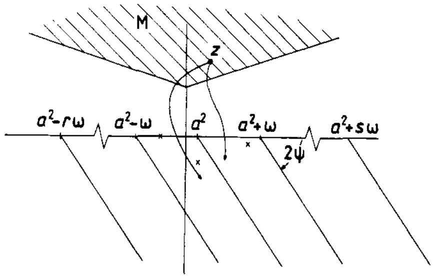

Figure 1. Analytic continuation in the complex z-plane of the resolvent $[z-H(\zeta)]^{-1}$. The spectrum of $H(\zeta)$ is given by the half-lines going off at an angle 2ψ ($\psi=\text{Im}\,\zeta$) and point eigenvalues of finite multiplicity (crosses). The domain of analyticity M can be extended to the whole open upper half-plane. Further continuations from a point $z\in M$ into different branches are indicated.

We note further that we cannot expect $R(z,\zeta)$, $\text{Im}\,z>0$, $\zeta\in I_{\alpha+}$ to have an analytic continuation to ζ with $\psi<0$. For, as soon as ψ becomes negative, an infinite number of half-lines from Σ will sweep over z and this will give rise to singularities.

5. Discussion

Although we shall be more specific in a future work concerned with actual applications, let us here briefly point out the connection between the present formalism and multiphoton ionisation processes. Suppose $V(r)$ possesses the properties (C) and suppose further that $H^{\text{at}}=T+V$ has a single non-degenerate bound state ϕ_0 with associated eigenvalue ε_0. Let this state be an s state. Then $\phi_0(\zeta)$ is still an eigenstate of $H^{at}(\zeta)=T(\zeta)+V(\zeta)$ at the eigenvalue ε_0. It may now happen that $H(\zeta)$, $\zeta\in I_+$ has a corresponding resonance eigenstate, i.e. an eigenstate $\phi(\zeta)$ with associated complex eigenvalue $E=\varepsilon_0+\Delta-i\Gamma=E_0-i\Gamma$. Since $\phi_0(\zeta)$ is the eigenvector of $H_1(\zeta)=H^{at}(\zeta)+a^2-\omega l_3$ (with eigenvalue ε_0+a^2) we can consider $\phi(\zeta)$ to be the perturbed eigenvector, related to $\phi_0(\zeta)$ under the perturbation $W(\zeta)=H(\zeta)-H_1(\zeta)=-2\boldsymbol{p}\cdot\boldsymbol{a}\exp(-\zeta)$. Since $W(\zeta)$ is $H_1(\zeta)$ bounded with zero relative bound it is indeed a well behaved perturbation. Let now the system be in the state ϕ_0 at time zero and let $\boldsymbol{A}(t)$ be switched on between time zero and time t after which time it is switched off again. The state vector at time t is then $\psi(t)=U(t)\phi_0=\exp(-i\omega l_3t)\exp(-i\bar{H}t)\phi_0$ so that the ionisation probability is

$$P_i=P_i(t)=1-|(\psi(t),\phi_0)|^2=1-|f(t)|^2 \tag{5.1}$$

with

$$\begin{aligned} f(t)&=(\exp(-i\omega l_3t)\exp(-i\bar{H}t)\phi_0,\phi_0)=(\exp(-i\bar{H}t)\phi_0,\phi_0)\\ &=(\exp[-iH(\zeta)t]\phi_0(\zeta),\phi_0(\bar{\zeta}))\\ &=-2\pi i\int_{-\infty+i\varepsilon}^{+\infty+i\varepsilon}dz\,\exp(-izt)([z-H(\zeta)]^{-1}\phi_0(\zeta),\phi_0(\bar{\zeta})). \end{aligned} \tag{5.2}$$

We now deform the contour as shown in figure 2. Then $f(t)$ becomes the sum of the residue in $z=E$ and a background contribution f_{bg}:

$$f(t)=f_0\exp[-i(E_0-i\Gamma)t]+f_{bg}(t). \tag{5.3}$$

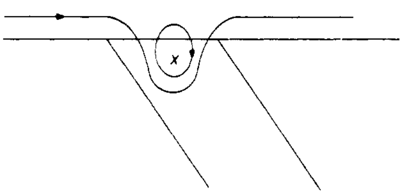

Figure 2. Deformation of the contour in order to evaluate the pole contribution from a complex pole in the lower half-plane.

If $f_{bg}(t)$ is small we thus find that ϕ_0 is approximately depopulated at a rate 2Γ. If $V(r)$ supports more bound states there will be more exponentially decaying contributions to $P_i(t)$. In that case it is more illuminating to consider the production of electrons in a certain energy interval ΔE. We expect that this process can be approximately described with a single rate constant, provided there is only a single bound state of $H_1(\zeta)$ in this interval. For a model where the field-free Hamiltonian possesses a single bound state we performed a calculation of the corresponding resonance and also of the energy spectrum of the emitted photo-ionised electron (Muller and Tip 1983). Due to the simplicity of the model a perturbation-free calculation was possible and the resonance could be followed in the complex plane up to fields in the order of one atomic unit (the field due to the nucleus an electron experiences in the first Bohr orbit in the hydrogen atom). The electronic energy spectrum shows peaks at energies $E_m=E_{ion}+m\hbar\omega$ (E_{ion} is the ionisation energy) with m such that $E_m>0$. In fact the term $m\hbar\omega$ enters the formalism as an eigenvalue of $\hbar\omega l_3$ and is related to the fact that energy can be removed from the radiation field by absorbing an integral number of photons, each having an angular momentum $\hbar$. This is brought out even more clearly in a second quantised formalism where, in the case of one circularly polarised field mode, the sum $N+l_3$ of the photon-number operator N and l_3 is a constant of the motion (see below for the second quantised formalism). It turns out that the above model nicely explains a number of features that were found experimentally in N-photon ionisation ($N \geqslant 11$) of Xenon atoms in intense laser fields (Kruit *et al* 1981, 1983).

We now discuss some related work.

5.1. *The* DC*–Stark case*

Here one studies the Hamiltonian

$$H = H^{\mathrm{at}} + E \sum_{j=0}^{N} e_j x_{jz} \tag{5.4}$$

which is (1.14) in the limit that $\omega \to 0$ and $E = \omega a$ (the electric field) constant. This type of Hamiltonian has been studied in great detail by various authors (Avron and Herbst 1977, Herbst 1979, Herbst and Simon 1981). Here we encounter another case where the complex-dilated Hamiltonian has no norm-resolvent limit but only a strong-resolvent one as the complex dilatation parameter becomes real (Herbst 1979). A technical point in common is the use of an explicit representation for the semi-group associated with the complex dilated free (i.e. $V=0$) Hamiltonian. The results differ dramatically, however. In the DC–Stark case the spectrum is empty for $0<|\mathrm{Im}\,\zeta|<\pi/3$, whereas here (appendix 2) we find an infinite set of parallel half-lines.

5.2. *Circularly polarised fields*

Circularly polarised fields have also been considered by Enns and Veselić (1983). These authors consider the same Hamiltonian as in the present work but for a larger class of potentials $V(r)$. They do not consider the possibility of complex dilatation but instead some scattering theoretical aspects. They also conjecture that for potentials $V(r)$ vanishing at infinity no bound states are left (i.e. at atom always ionises when it stays in the field indefinitely long). In a second quantised version of the theory (Grossmann and Tip 1980) it was found for hydrogen that an infinite set of negative energy bound states, accumulating in zero, exists. On the other hand it was found that the photo-ionisation probability tends to one in the limit of increasing field strength, provided that positive energy eigenvalues, if they exist at all, are restricted to a bounded region of the positive real axis.

5.3. *Linearly polarised fields*

In the general case of a self-adjoint Hamiltonian $H(t)$ acting in $\mathscr{H}$ and periodic in time with period $2\pi/\omega$, the time-evolution operator $U(t)=U(t,0)$ can be represented in the Floquet form $U(t)=W(t)\exp(-\mathrm{i}H^{\mathrm{Fl}}t)$, where H^{Fl} is defined by $\exp(-2\pi\mathrm{i}H^{\mathrm{Fl}}/\omega)=U(2\pi/\omega)$ and the unitary operator $W(t)$ is periodic in time with period $2\pi/\omega$. It follows that

$$-\mathrm{i}\partial_t W(t) - W(t)H^{\mathrm{Fl}} = -H(t)W(t). \tag{5.5}$$

The usual procedure is to consider this equation on an enlarged Hilbert space (Sambe 1973, Howland 1974, 1979; see also the pioneering work by Shirley (1965)). Thus let $t = x_0$ and let $p_0 = -i\partial_{x_0}$ on $\mathcal{H}_0 = L^2([0, 2\pi/\omega], dx_0)$ with periodic boundary conditions (so that $\sigma(p_0) = \{n\omega | n \in \mathbb{Z}\}$). Then on $\tilde{\mathcal{H}} = \mathcal{H}_0 \otimes \mathcal{H}$, (5.5) leads to the equation

$$p_0 W(x_0) - W(x_0)p_0 - W(x_0)H^{\mathrm{Fl}} = -H(x_0)W(x_0), \tag{5.6}$$

or, since $W(x_0)$ is unitary on $\tilde{\mathcal{H}}$,

$$W(x_0)^{-1}[p_0 + H(x_0)]W(x_0) = p_0 + H^{\mathrm{Fl}} = p_0 \otimes I + I_0 \otimes H^{\mathrm{Fl}}. \tag{5.7}$$

A similar formula for the corresponding unitary operators (so that no domain problems can arise) is given by Yajima (1982, equation (1.6)). It follows that $\tilde{H} = p_0 + H(x_0)$ and $p_0 + H^{\mathrm{Fl}}$ have the same spectrum. The transformation generated by $W(x_0)$ leads to a very special reduction of $\tilde{H}$ with a trivial part p_0 in H_0 and H^{Fl} in the original Hilbert space. For circularly polarised fields $W(x_0) = \exp(-i\omega l_3 x_0)$ and H^{Fl} are explicitly known and one can study H^{Fl} directly. Since $W(x_0)$ is dilatation invariant it is immaterial whether one studies the complex dilatation of H^{Fl} or of $\tilde{H}$.

In the linearly polarised case no general expressions for $W(x_0)$ and H^{Fl} seem to exist and calculations have been performed in terms of the explicitly known operator $\tilde{H}$ (Manakov *et al* 1976, 1978, Brodsky 1979). Although resonances are considered in these treatments, the complex dilatation method was not used. The complex dilatation theory for $\tilde{H}$ has recently been developed by Yajima (1982) and Yajima and Graffi (1983). It is interesting to note that the Kramers transformation (Kramers 1950), which shifts the field dependence of the Hamiltonian to the potential, plays an important role in many treatments. It seems that Brodsky (1979) was the first to realise that this transformation leads to compactness properties. It was used again by Grossmann and Tip (1980) in a second quantised version, by Yajima (1982; see also Kitada and Yajima 1982) and in the present work (equation (2.1)).

In all cases mentioned the idea behind its use is to obtain a relatively compact perturbation of some zero-order Hamiltonian with known spectrum.

Yajima also considers the perturbation expansion in powers of the field strength μ for the resonance eigenvalues λ of the dilated Hamiltonian which originate from the eigenvalues $\lambda_0 < 0$ of the field-free 'atomic' Hamiltonian. Under certain conditions on the potential he finds that for almost every $\omega > 0$ the leading term in $\mathrm{Im}\,\lambda$ for small μ is proportional to μ^{2n_0}, where n_0 is the smallest integer such that $\lambda_0 + n_0\omega > 0$. Although not mentioned by Yajima the exceptions to the rule can occur if there is a second eigenvalue λ_0', $\lambda_0 < \lambda_0' < 0$ and $\omega = \lambda_0' - \lambda_0$. If, for example, $n_0 = 2$ and $\omega = \lambda' - \lambda$ then $\mathrm{Im}\,\lambda \sim \mu^2$ instead of μ^4, provided the matrix elements of the field term in the 'atomic' Hamiltonian between the eigenstates associated with λ_0 and λ_0', respectively, are non-zero. (In terms of $\tilde{H}$ we are dealing with a degenerate eigenvalue whose degeneracy is lifted by the field term in $\tilde{H}$). Yajima's formalism of course also applies to the case of circularly polarised radiation fields. Since the field term in $\tilde{H}$ is different the positions of the resonances, although originating from the same eigenvalues, will in general deviate from those in the case of linear polarisation.

5.4. Single field mode in second quantisation

Many processes associated with atoms in radiation fields can be described equally well by means of a semiclassical approach (time-dependent external field) or in terms of a second quantised formalism. In the second case the field intensity enters the formalism through the photon occupation number in the initial state (in the product Hilbert space for atom and field). A complex dilatation formalism for hydrogen atoms in a single field mode was developed by Grossmann and Tip (1980). One basic difference with the semiclassical approach is that, due to the confining properties of the free-field Hamiltonian, the Hamiltonian is bounded from below. This is an important feature in connection with the extension of the dilatation formalism to many-electron atoms. The reason is that in the existing formulation (Balslev and Combes 1971, Simon 1972) use is made of the sectoriality properties of the various channel Hamiltonians. In the semiclassical approach both $H^{\mathrm{Fl}}(\zeta)$ (in the circularly polarised case) and $\tilde{H}(\zeta)$ do not possess this property, whereas in the second quantised case the sectoriality property holds and the extension is straightforward.

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Appendix 1

According to (2.6) we have

$$\Phi(r)=\begin{cases}1 & 0\leqslant r\leqslant\rho,\\ [1+(r-\rho)^2]^{-\alpha}, & \alpha\geqslant 1, r>\rho.\end{cases} \tag{A1.1}$$

Thus

$$\begin{aligned}\Psi(r)&\equiv\ln\Phi(r)=-\alpha\ln[1+(r-\rho)^2]\chi_{(\rho,\infty)}(r),\\ \boldsymbol{c}(r)&=\partial_{\boldsymbol{x}}\Psi(r)=-2\alpha(r-\rho)[1+(r-\rho)^2]^{-1}\chi_{(\rho,\infty)}(r)\boldsymbol{e}_x,\\ d(r)&=\partial_{\boldsymbol{x}}^2\Psi(r)=\{-2\alpha[1-(r-\rho)^2][1+(r-\rho)^2]^{-2}\\ &\qquad-(\alpha/r)(r-\rho)[1+(r-\rho)^2]^{-1}\}\chi_{(\rho,\infty)}(r),\end{aligned} \tag{A1.2}$$

where $\chi_{a,b)}(\cdot)$ is the characteristic function of the interval (a,b) and $\boldsymbol{e}_x=\boldsymbol{x}/|\boldsymbol{x}|$.

Let A be densely defined, $f\in\mathscr{D}(A)\cap\mathscr{D}(A^*)$ and $\lambda>0$. Then

$$\begin{aligned}0\leqslant\|[\lambda\sqrt{2}A\pm(\lambda\sqrt{2})^{-1}]f\|^2\Rightarrow|((A+A^*)f,f)|&\leqslant 2\lambda^2\|Af\|^2+(2\lambda^2)^{-1}\|f\|^2\\ &\leqslant(\lambda\sqrt{2}\|Af\|+(\lambda\sqrt{2})^{-1}\|f\|)^2,\end{aligned}$$

so that for $A=B^*B$, B densely defined,

$$\|Bf\|\leqslant\lambda\|B^*Bf\|+(2\lambda)^{-1}\|f\|. \tag{A1.3}$$

Since, for $f\in\mathscr{S}$, $\Phi Tf=\exp(\Psi)T\exp(-\Psi)\Phi f=(\boldsymbol{p}+\mathrm{i}\boldsymbol{c})^2\Phi f$, we have

$$\|T\Phi f\|=\|[\Phi T+\Phi(c^2-d)-2\mathrm{i}\boldsymbol{c}\cdot\boldsymbol{p}\Phi]f\|\leqslant\|\Phi Tf\|+\|\Phi(c^2-d)\|_\infty\|f\|+2\|\boldsymbol{c}\cdot\boldsymbol{p}\Phi f\|.$$

Next, using (A1.3),

$$\|c\cdot p\Phi f\|\leq\sum_{j=1}^{3}\|c_j\|_\infty\|p_j\Phi f\|\leq 3\|c\|_\infty\|p\Phi f\|$$
$$\leq 3\|c\|_\infty[\lambda_1\|T\Phi f\|+(2\lambda_1)^{-1}\|\Phi f\|]$$
$$\leq 3\|c\|_\infty\lambda_1\|T\Phi f\|+[3\|c\|_\infty/(2\lambda_1)]\|f\|$$

where $h=|\boldsymbol{h}|$ and $\lambda_1>0$ arbitrary. It follows that for sufficiently small λ_1

$$\|T\Phi f\|\leq(1-3\|c\|_\infty\lambda_1)^{-1}\{\|\Phi Tf\|+[\|\Phi(c^2-d)\|_\infty+3\|c\|_\infty/(2\lambda_1)]\|f\|\}$$
$$=(1+\delta)\|\Phi Tf\|+b'(\delta)\|f\| \tag{A1.4}$$

with arbitrarily small positive δ.

Now, for $\mu\in\mathbb{C}$,

$$\|\Phi Tf\|\leq\|\Phi(T-\mu l_3)f\|+|\mu|\|\Phi l_3 f\|\leq\|(T-\mu l_3)f\|+|\mu|\|\Phi l_3 f\|. \tag{A1.5}$$

Since l_3 commutes with $\Phi^{1/2}$ we obtain, using (A1.3) twice,

$$\|\Phi l_3 f\|=\|\Phi^{1/2}(x_1p_2-x_2p_1)\Phi^{1/2}f\|\leq\|\Phi^{1/2}x_1\|_\infty\|p_2\Phi^{1/2}f\|+\|\Phi^{1/2}x_2\|_\infty\|p_1\Phi^{1/2}f\|$$
$$\leq 2\|\Phi^{1/2}r\|_\infty\|p\Phi^{1/2}f\|$$
$$\leq 2\|\Phi^{1/2}r\|_\infty[\lambda_2\|\Phi^{1/2}T\Phi^{1/2}f\|+(2\lambda_2)^{-1}\|f\|]$$
$$=2\|\Phi^{1/2}r\|_\infty\{\lambda_2\|[T\Phi+\mathrm{i}c\cdot p\Phi+(\tfrac{1}{2}d-\tfrac{1}{4}c^2)\Phi]f\|+(2\lambda_2)^{-1}\|f\|\}$$
$$\leq 2\|\Phi^{1/2}r\|_\infty[\lambda_2\|T\Phi f\|+3\lambda_2\|c\|_\infty\|T\Phi f\|+3\lambda_2\|c\|_\infty\tfrac{1}{2}\|\Phi f\|$$
$$+\lambda_2\|(\tfrac{1}{2}d-\tfrac{1}{4}c^2)\Phi\|_\infty\|f\|+(2\lambda_2)^{-1}\|f\|]$$
$$=\lambda_2k_1\|T\Phi f\|+(\lambda_2k_2+\lambda_2^{-1}k_3)\|f\| \tag{A1.6}$$

where k_1, k_2 and k_3 are positive constants. Combining (A1.4), (A1.5) and (A1.6) we now have

$$\|T\Phi f\|\leq(1+\delta)\|(T-\mu l_3)f\|+b'(\delta)\|f\|+(1+\delta)\lambda_2k_1|\mu|\|T\Phi f\|$$
$$+(1+\delta)(\lambda_2k_2+\lambda_2^{-1}k_3)|\mu|\|f\|.$$

Let now $\lambda_2=\delta[(1+\delta)(1+2\delta)k_1|\mu|]^{-1}$. Then

$$\|T\Phi f\|\leq(1+2\delta)\|(T-\mu l_3)f\|+b(\delta)\|f\| \tag{A1.7}$$

which is (2.8) if we set $2\delta=\varepsilon$ and $\mu=\omega$. We now show that there is an interval $[0,\psi_3]$, $0\leq\psi_3<\pi/4$, such that for $\psi\in[0,\psi_3]$ and $f\in\mathscr{S}$

$$\|T\Phi f\|\leq k_1\|H_0(\boldsymbol{a},\mathrm{i}\psi)f\|+k_2\|f\| \tag{A1.8}$$

with k_1 and k_2 independent of ψ. Since

$$\cos 2\psi[p^2-(\omega/\cos 2\psi)l_3]f=[H_0(\boldsymbol{a},\mathrm{i}\psi)+2\boldsymbol{a}\cdot\boldsymbol{p}\,\mathrm{e}^{-\mathrm{i}\psi}+\mathrm{i}p^2\sin 2\psi+a^2]f,$$

we have, according to (A1.5),

$$\|\Phi Tf\|\leq(\cos 2\psi)^{-1}\|\Phi[H_0(\boldsymbol{a},\mathrm{i}\psi)+2\boldsymbol{a}\cdot\boldsymbol{p}\,\mathrm{e}^{-\mathrm{i}\psi}+\mathrm{i}p^2\sin 2\psi+a^2]f\|+(\omega/\cos 2\psi)\|\Phi l_3 f\|$$
$$\leq(\cos 2\psi)^{-1}\|H_0(\boldsymbol{a},\mathrm{i}\psi)f\|+\tan 2\psi\|\Phi Tf\|+(a^2/\cos 2\psi)\|f\|$$
$$+(\omega/\cos 2\psi)\|\Phi l_3 f\|+2(\cos 2\psi)^{-1}\|\Phi\boldsymbol{a}\cdot\boldsymbol{p}f\|, \tag{A1.9}$$

so that

$$\|\Phi Tf\| \leq (\cos 2\psi - \sin 2\psi)^{-1}(\|H_0(\boldsymbol{a}, \mathrm{i}\psi)f\| + a^2\|f\| + \omega\|\Phi l_3 f\| + 2\|\Phi \boldsymbol{a}\cdot \boldsymbol{p}f\|]$$
$$\leq K[\|H_0(\boldsymbol{a}, \mathrm{i}\psi)f\| + a^2\|f\| + \omega\|\Phi l_3 f\| + 2\|\Phi \boldsymbol{a}\cdot \boldsymbol{p}f\|] \tag{A1.10}$$

for $0 \leq \psi \leq \psi_3 < \pi/4$ (K is a constant).

Since ($\lambda_3 > 0$)

$$\|\Phi \boldsymbol{a}\cdot \boldsymbol{p}f\| = \|\boldsymbol{a}\cdot(\boldsymbol{p}+\mathrm{i}\boldsymbol{c})\Phi f\| \leq \|\boldsymbol{p}\cdot \boldsymbol{a}\Phi f\| + \|\boldsymbol{c}\cdot \boldsymbol{a}\Phi\|_\infty\|f\| \leq 2a\|p\Phi f\| + \|\boldsymbol{c}\cdot \boldsymbol{a}\Phi\|_\infty\|f\|$$
$$\leq 2a\lambda_3\|T\Phi f\| + (a/\lambda_3 + \|\boldsymbol{c}\cdot \boldsymbol{a}\Phi\|_\infty)\|f\|. \tag{A1.11}$$

Combining (A1.5), (A1.10), (A1.11) and (A1.6) we obtain (A1.8) by taking δ, λ_2 and λ_3 sufficiently small.

Appendix 2

Let $\boldsymbol{A}(t)$ be given by (1.2) and let $\zeta \in \mathbb{C}$. Then $H_0(\zeta, t) = [\boldsymbol{p}\exp[-\zeta] - \boldsymbol{A}(t)]^2$ with domain $\mathscr{D}(T)$ is closed and the corresponding evolution equation

$$\partial_t U_0(\zeta, t) = -\mathrm{i}H_0(\zeta, t)U_0(\zeta, t), \qquad U_0(\zeta, 0) = 1, \tag{A2.1}$$

has the unique solution

$$U_0(\zeta, t) = \exp\left(-\mathrm{i}\int_0^t \mathrm{d}s\, H_0(\zeta, s)\right)$$
$$= \exp(-\mathrm{i}\{[T(\zeta) + a^2]t - \{2a\exp[-\zeta]/\omega)[\sin\omega t p_1 + (1-\cos\omega t)p_2]\}). \tag{A2.2}$$

For $\zeta \in [0, \pi/2)$ we have

$$\|U_0(\zeta, t)\| = \exp[-\sin 2\psi(\boldsymbol{p}\exp(-\theta) - \boldsymbol{c})^2 t]\exp\{\tfrac{1}{2}a^2\tan\psi[\sin\tfrac{1}{2}\omega t/(\tfrac{1}{2}\omega t)]^2\}$$
$$\leq \exp(\tfrac{1}{2}a^2\tan\psi t), \tag{A2.3}$$

where

$$\boldsymbol{c} = \{a\sin\omega t/2\omega\cos\psi), a(1-\cos\omega t)/2\omega\cos\psi), 0\}.$$

Let

$$\hat{U}_0(\zeta, t) = \exp(-\mathrm{i}\omega l_3 t)\exp(-\mathrm{i}\bar{H}_0(\boldsymbol{a}_0, \zeta)t), \qquad \operatorname{Im}\zeta \in [0, \pi/2).$$

Proposition. $U_0(\zeta, t) = \hat{U}_0(\zeta, t)$.

Proof. For $\zeta \in I_+$ and $f \in \mathscr{D}_0$, $\exp[-\mathrm{i}H_0(\boldsymbol{a}, \zeta)t]f \in \mathscr{D}_0$ and, since $\exp(-\mathrm{i}\omega l_3 t)\mathscr{D}_0 = \mathscr{D}_0$, $\hat{U}_0(\zeta, t)f \in \mathscr{D}_0$. Let now $\zeta = \theta$ be real. In the following no generality is lost by taking $\theta = 0$. Referring to § 2 we have

$$\exp[-\mathrm{i}\bar{H}_0(\boldsymbol{a})t] = M\exp(-\mathrm{i}\bar{H}_0 t)M^{-1} = M\exp(-\mathrm{i}a^2 t)\exp(-\mathrm{i}Tt)\exp(\mathrm{i}\omega l_3 t)M^{-1} \tag{A2.4}$$

with $M = \exp(\mathrm{i}ap_2/\omega)$. From (A2.4) it is clear that $\exp[-\mathrm{i}\bar{H}_0(\boldsymbol{a})t]$ commutes with $(1+T)^{-1}$ and consequently $\exp[-\mathrm{i}\bar{H}_0(\boldsymbol{a})t]\mathscr{D}(T) = \mathscr{D}(T)$. Proceeding formally we have for $f \in \mathscr{D}_0$

$$\begin{aligned}\|l_3 \exp[-i\bar{H}_0(\boldsymbol{a})t]f\| &= \|\exp[i\bar{H}_0(\boldsymbol{a})t]l_3 \exp[-i\bar{H}_0(\boldsymbol{a})t]f\| \\ &= \|M \exp(-i\omega l_3 t)\exp(iTt)M^{-1}l_3 M \exp(-iTt)\exp(i\omega l_3 t)M^{-1}f\| \\ &= \|M \exp(-i\omega l_3 t)(l_3 - ap_1/\omega)\exp(i\omega l_3 t)M^{-1}f\| \\ &= M[l_3 - (a/\omega)(p_1 \cos\omega t + p_2 \sin\omega t)]M^{-1}f\| \\ &= \|\{l_3 + (a/\omega)[p_1(1-\cos\omega t) - p_2 \sin\omega t]\}f\| < \infty \qquad \text{(A2.5)}\end{aligned}$$

and this result becomes exact by reading (A2.5) in reverse order. We conclude that $\exp[-i\bar{H}_0(\boldsymbol{a})t]$ maps $\mathscr{D}_0$ into itself. Now, for $f \in \mathscr{D}_0$ and $\operatorname{Im}\zeta \in [0, \pi/2]$

$$\begin{aligned}\partial_t \hat{U}_0(\zeta, t)f &= -i\exp(-i\omega l_3 t)[\omega l_3 + \bar{H}_0(\boldsymbol{a}, \zeta)]\exp[-i\bar{H}_0(\boldsymbol{a}, \zeta)t]f \\ &= -i\exp(-i\omega l_3 t)[\boldsymbol{p}\exp(-\zeta) - \boldsymbol{a}]^2 \exp(i\omega l_3 t)\hat{U}_0(\zeta, t)f \\ &= -iH_0(\zeta, t)\hat{U}_0(\zeta, t)f.\end{aligned}$$

Since (A2.1) has a unique solution and both $U_0(\zeta, t)$ (see A2.3) and $\hat{U}_0(\zeta, t)$ are bounded, it follows from the result $U_0(\zeta, t)f = \hat{U}_0(\zeta, t)f$ for $f \in \mathscr{D}_0$ that $U_0(\zeta, t) = \hat{U}_0(\zeta, t)$ since $\mathscr{D}_0$ is dense.

It follows that

$$\begin{aligned}\exp[-i\bar{H}_0(\boldsymbol{a}, \zeta)t] &= \exp(i\omega l_3 t)U_0(\zeta, t) \\ &= \exp[-i(\bar{H}_0(\zeta) + a^2)t]\exp\{i[2a\exp(-\zeta)/\omega][p_1 \sin\omega t + p_2(1-\cos\omega t]\} \qquad \text{(A2.6)}\end{aligned}$$

so that for $\operatorname{Im}\zeta = \psi \in [0, \pi/2]$, $\operatorname{Im} z > \frac{1}{2}a^2 \tan\psi$ (see 3.5).

$$\begin{aligned}[z - \bar{H}_0(\boldsymbol{a}, \zeta)]^{-1} &= -i\int_0^\infty dt\, \exp[i(z - \bar{H}_0(\zeta) - a^2)t]\exp\{i[2a\exp(-\zeta)/\omega] \\ &\quad \times [p_1 \sin\omega t + p_2(1-\cos\omega t)]\}. \qquad \text{(A2.7)}\end{aligned}$$

Since the last exponential is periodic in t with period $2\pi/\omega$ we have

$$\begin{aligned}[z - \bar{H}_0(\boldsymbol{a}, \zeta)]^{-1} &= -i\sum_{n=0}^{\infty}\exp[i(z - \bar{H}_0(\zeta) - a^2)(2\pi n/\omega)]\int_0^{2\pi/\omega} dt\, \exp[i(z - \bar{H}_0(\zeta) - a^2)t] \\ &\quad \times \exp\{i[2a\exp(-\zeta)/\omega][p_1 \sin\omega t + p_2(1-\cos\omega t)]\} \\ &= -i\{1 - \exp[(2\pi i/\omega)(z - \bar{H}_0(\zeta) - a^2)]\}^{-1} \\ &\quad \times \int_0^{2\pi/\omega} dt\, \exp(izt)\exp(i\omega l_3 t)U_0(\zeta, t). \qquad \text{(A2.8)}\end{aligned}$$

Let

$$F(z, \zeta) = \{1 - \exp(2\pi i/\omega)[z - \bar{H}_0(\zeta) - a^2]\}^{-1}. \qquad \text{(A2.9)}$$

Its reduction to $\mathscr{H}_m$ is

$$F_m(z,\zeta)=(1-\exp\{(2\pi \mathrm{i}/\omega)[z-T_m(\zeta)+m\omega-a^2]\})^{-1}$$
$$=(1-\exp\{(2\pi \mathrm{i}/\omega)[z-T_m(\zeta)-a^2]\})^{-1},$$

so that

$$F(z,\zeta)=(1-\exp\{(2\pi \mathrm{i}/\omega)[z-T(\zeta)-a^2]\})^{-1}. \tag{A2.10}$$

From (A2.10) it is seen that $F(z,\zeta)$ is a bounded-operator-valued analytic function of $z\in\mathbb{C}$, except for the set of half-lines

$$\Sigma=\Sigma(a,\zeta)=\Sigma(a,\psi)=\{z=a^2+\lambda\,\exp(-2\mathrm{i}\psi)+k\omega,\ \lambda\in[0,\infty],\ k\in\mathbb{Z}\}. \tag{A2.11}$$

We note that $\Sigma=\mathbb{R}$ for $\zeta=\theta$ real and that $F(z,\zeta)^{-1}$ and $F^*(z,\zeta)^{-1}$ do not have a bounded inverse for $z\in\Sigma$. Since $\|U_0(\zeta,t)\|$ is bounded by $\exp(\frac{1}{2}a^2t\tan\psi)$ it follows that

$$G(z,\zeta)=\int_0^{2\pi/\omega}\mathrm{d}t\,\exp(\mathrm{i}zt)\exp(\mathrm{i}\omega l_3t)U_0(\zeta,t) \tag{A2.12}$$

is a bounded-operator-valued analytic function of z. It follows that for $\zeta\in I_+$ the right-hand side of (A2.8) is a bounded-operator-valued analytic function of $z\in\Sigma'=\mathbb{C}/\Sigma$. Since for such ζ, Σ' is a connected region in $\mathbb{C}$ it follows that $\Sigma'\subset\rho(H_0(\boldsymbol{a},\zeta))$. Since $([z-\bar{H}_0(\boldsymbol{a},\zeta)]^{-1})^*=\mathrm{i}G^*(z,\zeta)F^*(z,\zeta)$ and $F^*(z,\zeta)^{-1}$ does not have a bounded inverse for $z\in\Sigma$ it follows that $\sigma(H_0(\boldsymbol{a},\zeta))=\Sigma$ and $\rho(H_0(\boldsymbol{a},\zeta))=\Sigma'$ for $\zeta\in I_+$. Thus

Theorem. Let $\zeta\in I_\pm$. Then $\sigma(H_0(\boldsymbol{a},\zeta))=\Sigma(a,\psi)$.

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