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1980 J. Phys. A: Math. Gen. 13 3381

(http://iopscience.iop.org/0305-4470/13/11/012)

J. Phys. A: Math. Gen. 13 (1980) 3381–3397. Printed in Great Britain

# Hydrogen atoms interacting with a quantised radiation mode

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Received 31 January 1980, in final form 19 May 1980

**Abstract.** A model consisting of a hydrogen atom coupled to a single quantised radiation mode in the long-wavelength approximation is studied mathematically. It is shown that the Hamiltonian $H$ for this model is dilatation analytic. This result makes it possible to describe various resonance phenomena associated with atoms in radiation fields by means of analytic continuation techniques. Furthermore, it is shown that $H$ possesses an infinite number of bound states with negative energy. Nevertheless the photoionisation probability tends to one with increasing field strength.

## 1. Introduction

The development of lasers capable of producing very intense monochromatic radiation fields has led to an increasing interest in the properties of atomic systems placed in such fields. A proper theoretical description of atomic processes in intense fields should preferably not be of a perturbative nature with respect to the atom–field interaction and/or the field intensity, in order to facilitate the study of the asymptotic behaviour of the various possible processes in the high field intensity limit.

In the present work we study, from the mathematical point of view, one of the simplest possible systems: a 'model' H-atom coupled to a single quantised radiation mode in the long-wavelength approximation. In this approach the field intensity comes in through the initial state of the radiation mode, but the properties of the Hamiltonian are independent of the field. This is different when the field is treated classically. Then the Hamiltonian is time-dependent and the notion of bound states becomes somewhat more complicated. We comment further on this matter in § 5. The model considered here can describe physical processes such as multi-photon ionisation phenomena and free–free transitions (see a recent review by Gavrila and van der Wiel (1978)). The scattering of photons from an atom is outside its scope, since asymptotically free photon wave-packets can only be constructed if a continuum of field modes is available. This drawback is inherent to all model systems pertaining to a finite or countably infinite number of radiation modes (e.g. in box-normalised radiation fields). A treatment of atomic systems coupled to a continuum of field modes, however, leads to complicated structures in terms of infinite tensor products even if infrared and ultraviolet cut-offs are made (Cook 1961, Blanchard 1969). If an atomic system is subjected to a strong single-mode laser field, then the initial field state will contain photon states with

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energies centred in a small band around the central laser frequency. It is then natural to approximate this situation by a single-mode model and to neglect all other radiation modes. A more precise description of this procedure would of course be desirable, but will probably have to wait until the rigorous theory for continua of field modes is more fully developed.

We also assume the atomic nucleus to be infinitely heavy and we discard the spin degrees of freedom. In addition, we replace the actual vector potential $\boldsymbol{A}(\boldsymbol{x})$ by its value at $\boldsymbol{x} = 0$, i.e. we make a long-wavelength approximation. This excludes the description of various physical processes. On the other hand, for laser frequencies in the optical region, the relevant parameter, atomic dimension/field wavelength, is of the order of $10^{-3}$ or smaller, so that such processes will be of lesser importance.

The present work is organised in the following way. In § 2 we define our model. Basically we deal with a system describing a fictitious particle in a five-dimensional configuration space. In three dimensions it feels a Coulomb attraction, whereas in the other two it is confined by a harmonic potential (see equations (2.10)). The latter, of course, originates from the field Hamiltonian (two dimensions since there are two possible polarisations). In principle, bound states can exist with positive energy (the sum of atomic and oscillator eigenvalues). The interaction between atom and field, however, can change this and in general such bound states can be expected to turn into resonances. One way of studying this mechanism is to use the machinery of dilatation analyticity (see Simon (1973) for the application to autoionising atomic states), and indeed one of our results is the applicability of the dilatation method to the present model (§§ 3 and 4). This gives some information about the spectral properties of the Hamiltonian for the model; results which are complemented in § 5 by showing that the coupling between atom and field does not wipe out all bound states. In fact, there is an infinite number of bound states with negative energy, in contradistinction with the DC–Stark effect case where no bound states survive. Still, one may expect ionisation probabilities to tend to unity with increasing field strength since, as also shown in § 5, the overlap between the above bound states and the initial states, usually encountered in multi-photon processes, tends to zero with increasing photon number in the initial state. The paper ends with a discussion section where, among other things, we point out some applications and generalisations. In summary, we have obtained the following results. The Hamiltonian of the model, $H$, is dilatation analytic. This property makes it possible to apply analytic continuation techniques to the description of photoionisation processes and similar phenomena such as free–free transitions. Secondly, $H$ possesses an infinite number of bound states. Nevertheless the photoionisation probability tends to unity with increasing field intensity (i.e. increasing occupation number of the initial field state).

Some recent related literature is Rosenberg (1979), where various other aspects of the same model are discussed, and Brodsky (1979), where the field is treated classically. The complex dilated harmonic oscillator, finally, has been considered earlier by van Winter (1980).

In the present work the notions relative boundedness and relative compactness occur frequently. The latter, in particular, is of considerable importance since relatively compact perturbations of an operator leave its essential spectrum, $\sigma_{\mathrm{ess}}$, invariant (the essential spectrum of an operator is its full spectrum with the exception of $\sigma_{\mathrm{d}}$, the discrete spectrum, i.e. the isolated eigenvalues with finite degeneracy). For a full treatment of these and other concepts used in the present paper we refer to Kato (1966) and Reed and Simon (1972, 1975, 1978).

## 2. Definition of the model

We consider an electron moving in an attractive Coulomb field (centred around the origin) and at the same time coupled to a quantised radiation mode. The Hamiltonian of this system is formally given by (in MKSA units)

$$H = (\hbar^2/2m)[\boldsymbol{p} - (e/\hbar)\boldsymbol{A}(\boldsymbol{x})]^2 + V(\boldsymbol{x}) + H^{\mathrm{f}} \tag{2.1}$$

where $\boldsymbol{x}$, $\boldsymbol{p} = -\mathrm{i}\,\partial_{\boldsymbol{x}}$, $e$ and $m$ are the electronic position vector, momentum (in units $\hbar$), charge and mass, respectively. $V(\boldsymbol{x})$ represents the Coulomb potential, $V(\boldsymbol{x}) = -Ze^2/(4\pi\epsilon_0|\boldsymbol{x}|)$ ($Z = 1$ for hydrogen) and $\boldsymbol{A}(\boldsymbol{x})$ is the vector potential in the Coulomb gauge. Its usual box-normalised form is

$$\boldsymbol{A}(\boldsymbol{x}) = [\hbar/(2\epsilon_0 L^3)]^{1/2} \sum_{k,\lambda} (\omega_k)^{-1/2}[a_{k\lambda} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}) + a^*_{k\lambda} \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})]\cdot \boldsymbol{e}_\lambda(\boldsymbol{k}). \tag{2.2}$$

Here $\epsilon_0$ is the dielectric constant, $\omega_k = c|\boldsymbol{k}|$, $\boldsymbol{k} = 2\pi\boldsymbol{n}/L$, $n_j = 0, \pm 1, \pm 2, \ldots, j = 1, 2, 3$. $a_{k\lambda}$ and $a^*_{k\lambda}$ are annihilation and creation operators obeying the commutation relations

$$[a_{k\lambda}, a^*_{k'\lambda'}] = \delta_{kk'}\delta_{\lambda\lambda'} \tag{2.3}$$

and $\boldsymbol{e}_\lambda(\boldsymbol{k})$, $\lambda = 1, 2$, are the two polarisation vectors orthogonal to $\boldsymbol{k}$ and to each other. The free field Hamiltonian $H^{\mathrm{f}}$ is given by

$$H^{\mathrm{f}} = \hbar \sum_{k,\lambda} \omega_k a^*_{k\lambda} a_{k\lambda}. \tag{2.4}$$

In our model only a single field mode is retained, i.e. in the summation over $\boldsymbol{k}$ in (2.2) and (2.4) all terms but one are dropped. Thus a single photon carries a momentum $\hbar\boldsymbol{k}$, whereas $L$ is the photon wavelength: $\omega L = 2\pi c$. We also make a long-wavelength (or dipole) approximation, that is, we replace $\boldsymbol{A}(\boldsymbol{x})$ by its value at $\boldsymbol{x} = 0$ so that now

$$\boldsymbol{A} = [\hbar/(2\epsilon_0\omega L^3)]^{1/2} \sum_{\lambda=1}^{2} (a_\lambda + a^*_\lambda)\boldsymbol{e}_\lambda. \tag{2.5}$$

We now express the creation and annihilation operators in terms of fictitious position and momentum operators $\boldsymbol{x}_2$ and $\boldsymbol{p}_2$. Since there are only two polarisation directions, the latter have only two components, which we take along the $X$ and $Y$ axes so that $\boldsymbol{k}$ is directed along the $Z$ axis:

$$x_{2\lambda} = \tfrac{1}{2}\mathrm{i}\sqrt{2}(a_\lambda - a^*_\lambda), \qquad p_{2\lambda} = \tfrac{1}{2}\sqrt{2}(a_\lambda + a^*_\lambda). \tag{2.6}$$

We introduce atomic units according to

$$\boldsymbol{x} = a_0\boldsymbol{x}_1, \qquad \boldsymbol{p} = a_0^{-1}\boldsymbol{p}_1, \qquad L = a_0 l, \qquad \omega = [\hbar/(ma_0^2)]\tilde{\omega},$$

where

$$a_0 = 4\pi\epsilon_0\hbar^2/(me^2) \qquad \text{and} \qquad \alpha = e^2/(4\pi\epsilon_0\hbar c)$$

are the Bohr radius and fine-structure constant, respectively. Thus

$$H = [\hbar^2/(ma_0^2)]\tilde{H},$$
$$\tilde{H} = \tfrac{1}{2}(\boldsymbol{p}_1 - \sigma\boldsymbol{p}_2)^2 + \tilde{V}(\boldsymbol{x}_1) + \tilde{\omega}[\tfrac{1}{2}(\boldsymbol{p}_2^2 + \boldsymbol{x}_2^2) - 1], \tag{2.7}$$

where

$$\sigma = \tilde{\omega}[\alpha^3/(2\pi^2)]^{1/2}, \qquad \tilde{V}(\boldsymbol{x}) = -Z/|\boldsymbol{x}|.$$

We note in passing that the addition of a specific second field mode, namely the one associated with opposite momentum ($-\hbar\boldsymbol{k}$ instead of $\hbar\boldsymbol{k}$), is easily incorporated. A convenient choice of field coordinates and momenta then results in a Hamiltonian of the form (2.7) with a second, independent, oscillator part added. Thus the study of its spectral properties directly reduces to that of (2.7).

It is a straightforward matter to establish the self-adjointness of $\tilde{H}$ on its natural domain. We do not go into this, but bring it to a different form by making a canonical transformation that removes the cross-term $\boldsymbol{p}_1 \cdot \boldsymbol{p}_2$ giving rise to a different coordinate dependence of $V$ (see, however, § 6.1). It consists of a simplified form of a well known type of transformation (bilinear in particle momentum and the Hertz vector) that goes back to Breit and Kramers (Kramers 1950). Thus with

$$U(\lambda) = \exp(-\mathrm{i}\lambda \boldsymbol{p}_1 \cdot \boldsymbol{x}_2), \qquad \lambda = \sigma/(\tilde{\omega} + \sigma^2), \tag{2.8}$$

we have (notation $\boldsymbol{p}_1 = \{p_{11}, p_{12}, p_{13}\}$)

$$\begin{aligned}\tilde{H}(\lambda) &= U(\lambda)\tilde{H}U(\lambda)^{-1} \\ &= \tfrac{1}{2}(1+\delta^2)^{-1}(p_{11}^2 + p_{12}^2) + \tfrac{1}{2}p_{13}^2 + V(\boldsymbol{x}_1 - \lambda \boldsymbol{x}_2) + \tilde{\omega}[\tfrac{1}{2}(1+\delta^2)\boldsymbol{p}_2^2 + \tfrac{1}{2}\boldsymbol{x}_2^2 - 1],\end{aligned} \tag{2.9}$$

where

$$\delta^2 = \sigma^2/\tilde{\omega} = \alpha^2/(\pi l), \qquad \text{so that} \qquad \lambda = \rho/(1+\delta^2)$$

with

$$\rho = [\alpha^3/(2\pi^2)]^{1/2}.$$

Although it is possible to carry through our further analysis starting from (2.9) (after some suitable scaling the only difference is a replacement of the central Coulomb potential by a potential having ellipsoidal equipotential surfaces), it is consistent with the assumptions made so far to neglect $\delta^2$ in this expression: we have already supposed the field wavelength to be large as compared with atomic dimensions, i.e. $l \gg 1$. But then $\delta^2 = \alpha^2/(\pi l) \ll l^{-1} \ll 1$. In this way, we finally arrive at the Hamiltonian (we delete the tildes from now on)

$$H = \tfrac{1}{2}\boldsymbol{p}_1^2 + V(\boldsymbol{x}_1 - \rho \boldsymbol{x}_2) + \omega[\tfrac{1}{2}(\boldsymbol{p}_2^2 + \boldsymbol{x}_2^2) - 1]. \tag{2.10}$$

In view of our further discussion it is convenient to write $H$ as

$$H = H_0 + V(\boldsymbol{x}_1 - \rho \boldsymbol{x}_2) \tag{2.11}$$

or as

$$H = H_1 + W(\boldsymbol{x}_1, \boldsymbol{x}_2) \tag{2.12}$$

where

$$\begin{aligned} H_0 &= \tfrac{1}{2}\boldsymbol{p}_1^2 + H^{\mathrm{osc}}, \qquad H^{\mathrm{osc}} = \omega[\tfrac{1}{2}(\boldsymbol{p}_2^2 + \boldsymbol{x}_2^2) - 1], \\ H_1 &= H^{\mathrm{at}} + H^{\mathrm{osc}}, \qquad H^{\mathrm{at}} = \tfrac{1}{2}\boldsymbol{p}_1^2 + V(\boldsymbol{x}_1), \\ W(\boldsymbol{x}_1, \boldsymbol{x}_2) &= V(\boldsymbol{x}_1 - \rho \boldsymbol{x}_2) - V(\boldsymbol{x}_1). \end{aligned} \tag{2.13}$$

Both in (2.7) and in (2.12) we encounter a system consisting of a hydrogen atom and a harmonic oscillator which interact through a coupling term. In (2.7) it is the 'Hughes–Eckart type' term, $\sigma \boldsymbol{p}_1 \cdot \boldsymbol{p}_2$, whereas in (2.12) it is the potential $W(\boldsymbol{x}_1, \boldsymbol{x}_2)$. The form

(2.12), however, has the advantage that $W$ possesses relative compactness properties, as will be discussed in § 4. The spectrum of $H_1$ can be simply described. It consists of sums of atomic ($\epsilon_n$) and oscillator ($l\omega$, $l = 0, 1, 2, \ldots$) eigenvalues $E_{nl} = \epsilon_n + l\omega$, as well as a continuous spectrum covering the positive real axis with branches starting at $l\omega$, $l = 0, 1, 2, \ldots$. Clearly there are many continuum-embedded eigenvalues, which are likely to turn into resonances under the perturbation $W$. A similar situation is encountered in dealing with atomic autoionising states where the Coulomb repulsion plays the role of $W$.

## 3. Dilatation analyticity and the harmonic oscillator

As a necessary preliminary for the study of the dilatation-analytic properties of the Hamiltonian (2.10), we discuss here these properties for the $n$-dimensional harmonic oscillator. The results are also relevant for other problems where harmonic oscillator Hamiltonians appear. Examples are systems with coupled scattering and confining channels, as found in molecular predissociation and non-relativistic quark-confinement models. Dilatation analyticity in its original form (Aguilar and Combes 1971) is centred around the notion of relatively compact potentials with respect to $\boldsymbol{p}^2$, $\boldsymbol{p} = -\mathrm{i}\partial_{\boldsymbol{x}}$ on $L^2(\mathbb{R}^n)$. Since the harmonic oscillator potential lacks this property, we need here a more general definition of dilatation analyticity.

The dilatation group on $L^2(\mathbb{R}^n)$ is the group

$$\{U(\theta)\} = \{\exp[\tfrac{1}{2}\mathrm{i}\theta(\boldsymbol{x}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{x})],\ \theta \in \mathbb{R}\} \tag{3.1}$$

of unitary operators. We have $(U(\theta)f)(\boldsymbol{x}) = \exp(n\theta/2) f(\mathrm{e}^{\theta}\boldsymbol{x})$ for $f \in L^2(\mathbb{R}^n)$.

*Definition.* Let $H$ be self-adjoint with domain $\mathscr{D} \subset L^2(\mathbb{R}^n)$, and suppose that $\mathscr{D}$ is invariant under $U(\theta)$ for each $\theta \in \mathbb{R}$, so that the family $\{H(\theta) = U(\theta)HU^{-1}(\theta),\ \theta \in \mathbb{R}\}$ is a family of self-adjoint operators with common domain. We shall say that $H$ is dilatation analytic and $\{H(\theta),\ \theta \in \mathscr{M}\}$ is a dilatation analytic family in an open set $\mathscr{M} \subset \mathbb{C}$ if $H(\theta)$ can be given a meaning for $\theta \in \mathscr{M} \subset \mathbb{C}$ such that $\{H(\theta),\ \theta \in \mathscr{M}\}$ is a self-adjoint holomorphic family of type A in Kato's sense (Kato 1966, ch 7).

Let the number operator $N$ on $L^2(\mathbb{R}^n)$ be given by

$$N = \tfrac{1}{2}(\boldsymbol{x}^2 + \boldsymbol{p}^2) - \tfrac{1}{2}n. \tag{3.2}$$

It represents the Hamiltonian of the $n$-dimensional isotropic harmonic oscillator modulo a multiplicative constant. Let $\{u_k(x),\ k = 1, 2, \ldots\}$ be the set of normalised one-dimensional harmonic oscillator eigenfunctions (Hermite functions). The eigenfunctions $u_l(\boldsymbol{x})$ ($l = \{l_1, l_2, \ldots, l_n\}$) and corresponding eigenvalues $\lambda_l$ of $N$ are then given by

$$u_l(\boldsymbol{x}) = \prod_{j=1}^{n} u_{l_j}(x_j), \qquad \lambda_l \equiv l = \sum_{j=1}^{n} l_j. \tag{3.3}$$

$N$ defines a self-adjoint operator on $L^2(\mathbb{R}^n)$ with domain $\mathscr{D}$. If we write the Hermite expansion of $f \in L^2(\mathbb{R}^n)$ as

$$f(\boldsymbol{x}) = \sum_l f_l u_l(\boldsymbol{x}), \tag{3.4}$$

then $\mathscr{D}$ consists of those $f$ for which $\Sigma_l\, l^2 |f_l|^2$ is finite.

*Proposition.* $\mathscr{D}$ is invariant under transformations of the dilatation group.

*Proof.* In order to keep the bookkeeping simple we sketch a proof for the one-dimensional case. We note that $u_l(\theta) = U(\theta)u_l$, $\theta$ real, is contained in $\mathscr{D}$ and, using recursion relations,

$$Nu_l(\theta) = A_l u_{l-2}(\theta) + B_l u_l(\theta) + C_l u_{l+2}(\theta) \tag{3.5}$$

where $A_l$, $B_l$ and $C_l$ are $O(l)$ (notation $u_l \equiv 0$, $l \leqslant 0$).
Now let $f \in \mathscr{D}$. Then

$$f(\theta) = U(\theta)f = \sum_{l=1}^{\infty} f_l u_l(\theta), \qquad f^m(\theta) = \sum_{l=1}^{m} f_l u_l(\theta). \tag{3.6}$$

Next we calculate $Nf^m(\theta)$ using (3.5). In view of the $O(l)$ property of $A_l$, $B_l$ and $C_l$, we find that ($K$ is a positive constant)

$$\|Nf^m(\theta) - Nf^n(\theta)\| \leqslant K \sum_{l=n-2}^{m+2} l^2 |f_l|^2.$$

Thus $Nf^m(\theta)$ is norm convergent, and since $N$ is closed it follows that $f(\theta) \in \mathscr{D}$. □
Let $N(\theta) = U(\theta)NU^{-1}(\theta)$. It has the explicit form

$$N(\theta) = \tfrac{1}{2}[\exp(2\theta)\boldsymbol{x}^2 + \exp(-2\theta)\boldsymbol{p}^2] - \tfrac{1}{2}n, \qquad \theta \in \mathbb{R}. \tag{3.7}$$

*Theorem.* $N$ is dilatation analytic. The members of the dilatation analytic family $\{N(\theta)\}$ are those for which $|\operatorname{Im}\theta| < \pi/4$.

*Proof.* We write $N(\theta) = \frac{1}{2}\exp(-2\theta)M - \frac{1}{2}n$, where $M = \exp(4\theta)\boldsymbol{x}^2 + \boldsymbol{p}^2 = \beta\boldsymbol{x}^2 + \boldsymbol{p}^2 = M(\beta)$, $\beta > 0$. We have to show that $\{M(\beta) | \beta \in \mathbb{C}\backslash(-\infty, 0]\}$ is a type-A family in Kato's sense. For $f \in \mathscr{D}$ we have

$$\begin{aligned}\|M(\beta)f\|^2 = {} & |\beta|^2\|\boldsymbol{x}^2 f\|^2 + \|\boldsymbol{p}^2 f\|^2 + \operatorname{Re}\beta[(\boldsymbol{x}^2 f, \boldsymbol{p}^2 f) + (\boldsymbol{p}^2 f, \boldsymbol{x}^2 f)] \\ & + \mathrm{i}\operatorname{Im}\beta[(\boldsymbol{x}^2 f, \boldsymbol{p}^2 f) - (\boldsymbol{p}^2 f, \boldsymbol{x}^2 f)].\end{aligned} \tag{3.8}$$

The identities

$$\begin{aligned} x_i^2 p_i^2 + p_i^2 x_i^2 &= \tfrac{1}{2}(x_i p_i + p_i x_i)^2 - \tfrac{3}{2}, \\ x_i^2 p_i^2 - p_i^2 x_i^2 &= 2\mathrm{i}(x_i p_i + p_i x_i), \end{aligned} \qquad i = 1, \ldots, n, \tag{3.9}$$

hold on $\mathscr{D}(N^2)$, the domain of $N^2$.

For such $f$ we can move the operators in the inner products in (3.8) from the right to the left, and using (3.9) we obtain, setting $\beta = \rho\exp(\mathrm{i}\psi)$,

$$\begin{aligned}\|M(\beta)f\|^2 = {} & \rho^2\|\boldsymbol{x}^2 f\| + \|\boldsymbol{p}^2 f\| + \tfrac{1}{2}\rho\cos\psi \sum_{i=1}^{n} ([x_i p_i + p_i x_i + 2\tan\psi]^2 f, f) \\ & + 4\rho\cos\psi \sum_{i>j} \|x_i p_j f\|^2 - [\rho n(3 + \sin^2\psi)/(2\cos\psi)]\|f\|^2.\end{aligned} \tag{3.10}$$

Since the right-hand side of (3.10) is well defined for $f \in \mathscr{D}$, we conclude that (3.10) holds for such $f$. Consequently we have

$$\rho^2\|\boldsymbol{x}^2 f\| \leqslant \|M(\beta)f\|^2 + [\rho n(3 + \sin^2\psi)/(2\cos\psi)]\|f\|^2 \tag{3.11}$$

for each $f \in \mathscr{D}$ and $|\psi| < \frac{1}{2}\pi$. Since $M(\beta)$, $\beta > 0$, is self-adjoint on $\mathscr{D}$, it follows from (3.11) that the operator $\gamma x^2$, $\gamma \in \mathbb{C}$, $|\gamma| < \beta$, is relatively bounded with relative bound smaller than one with respect to $M(\beta)$. Thus (see Kato 1966, ch 7) $\{M(\beta+\gamma) | |\gamma| < \beta\}$ is a self-adjoint type-A family. Since $\beta$ can be chosen arbitrarily large, we see that the analyticity domain $\mathscr{M}$ of $\{M(\zeta) | \zeta \in \mathscr{M}\}$ contains the open right half plane. Now let $\zeta_0 \in \mathbb{C}$, $\operatorname{Re} \zeta_0 > 0$, $\operatorname{Im} \zeta_0 > 0$. Then $M(\zeta_0)$ is a member of our family and we note that $\gamma x^2$, $|\gamma| < |\zeta_0|$, is $M(\zeta_0)$-bounded with relative bound smaller than one. Thus the analyticity domain can be extended to the open circle around $\zeta_0$ with radius $|\gamma|$. Making $\operatorname{Im} \zeta_0$ large and $\operatorname{Re} \zeta_0$ small, we thus reach each point in the open second quadrant in $\mathbb{C}$, as well as the positive imaginary axis except for the origin. A similar reasoning applies to the third quadrant and the negative imaginary axis. Thus $\mathscr{M} \supset \mathbb{C} \backslash (-\infty, 0]$, which proves the first part of the theorem.

Since we are dealing with a type-A family and $N$ has compact resolvent, it follows (Kato 1966, ch 7, theorem 2.4) that $N(\theta)$ has compact resolvent, and consequently its spectrum consists of isolated eigenvalues of finite multiplicity (Kato 1966, ch 3, theorem 6.29). A standard argument based upon the unitarity of $U(\theta)$, $\theta$ real, and the analyticity of isolated eigenvalues as a function of $\theta$ (Reed and Simon 1978, proof of theorem 13.36) results in the invariance of the eigenvalues of $N$ under complex dilatation transformations. □

The analyticity domain $|\operatorname{Im} \theta| < \pi/4$ is indeed the maximal one. The eigenfunctions of $N$ consist of polynomials times $\exp(-\frac{1}{2}x^2)$, and they lose the square integrability property if $|\operatorname{Im} \theta| = \pi/4$ in $\exp(-\frac{1}{2}e^{2\theta}x^2)$.

## 4. Spectral properties of the dilated Hamiltonian

In this section we study the spectral properties of the Hamiltonian (2.10). We start with $H_0 = \frac{1}{2}p_1^2 + H^{\mathrm{osc}}$ as given by (2.13). Thus let $T_1 = \frac{1}{2}p_1^2$ be the electronic kinetic energy operator, self-adjoint on the domain $\mathscr{D}_1 \subset \mathscr{H}_1 = L^2(\mathbb{R}^3)$. Since $\mathscr{D}_1$ is invariant under dilatation transformations (Aguilar and Combes 1971), we have for real $\theta$ $T_1(\theta) = U(\theta) T_1 U^{-1}(\theta) = \exp(-2\theta) T_1$, which operator remains closed on $\mathscr{D}_1$ for every $\theta \in \mathbb{C}$. Further, let $H^{\mathrm{osc}} = \omega N$ be the two-dimensional harmonic oscillator Hamiltonian, self-adjoint on $\mathscr{D}_2 \subset \mathscr{H}_2 = L^2(\mathbb{R}^2)$. In § 3 we found that $H^{\mathrm{osc}}$ is dilatation analytic and that $H^{\mathrm{osc}}(\theta)$, $|\operatorname{Im} \theta| < \pi/4$, is closed on $\mathscr{D}_2$. We now set (for operator tensor products see Reed and Simon (1972, ch 8.10))

$$H_0(\theta) = T_1(\theta) \otimes I_2 + I_1 \otimes H^{\mathrm{osc}}(\theta), \qquad |\operatorname{Im} \theta| < \pi/4. \tag{4.1}$$

This operator is defined on $\bigvee(\mathscr{D}_1 \otimes \mathscr{D}_2)$, the set of finite linear combinations of elements of $\mathscr{D}_1 \otimes \mathscr{D}_2$.

Since $T_1(\theta)$ and $H^{\mathrm{osc}}(\theta)$ are strictly $m$-sectorial, it follows that the spectrum of the closure $\bar{H}_0(\theta)$ of $H_0(\theta)$ is generated by all possible sums of points of the spectra of $T_1(\theta)$ and $H^{\mathrm{osc}}(\theta)$ (Reed and Simon 1978, ch 13.9). The spectrum of $T_1(\theta)$ consists of a half-line starting at the origin and going off at an angle $-2\psi$ ($\psi = \operatorname{Im} \theta$) with respect to the positive real axis. Consequently, the spectrum of $\bar{H}_0(\theta)$ consists of a set of such half-lines, each starting at a harmonic oscillator eigenvalue $l\omega$, $l = 0, 1, 2, \ldots$ (see figure 1). We now show that $\mathscr{D}(\theta)$, the domain of $\bar{H}_0(\theta)$, is independent of $\theta$.

*Lemma 1.* Let $A_i$ be closed with domain $\mathscr{D}_i \subset \mathscr{H}_i$, $i = 1, 2$, and let $B$ be closed on a

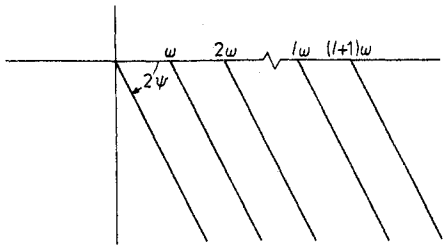


**Figure 1.** The spectrum of $\bar{H}_0(\theta)$ in the complex energy plane. It consists of a set of half-lines going off at an angle $-2\psi$.

domain $\mathscr{D}(B)$, $\mathscr{D}_2 \supset \mathscr{D}(B) \supset \mathscr{H}_2$. Let $\bar{A}$ be the closure of $A = A_1 \otimes I_2 + I_1 \otimes A_2$ and $\mathscr{D}(\bar{A})$ its domain. Suppose that $B$ is $A_2$-bounded with relative bound $a < 1$. Then $\bar{B}$, the closure of $I_1 \otimes B$, has domain $\mathscr{D}(\bar{B}) \supset \mathscr{D}(\bar{A})$ and $\bar{B}$ is $\bar{A}$-bounded with the same relative bound $a$.

*Proof.* The dense set $\bigvee(\mathscr{D}_1 \otimes \mathscr{D}_2) \subset \mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$ is contained in both $\mathscr{D}(\bar{A})$ and $\mathscr{D}(\bar{B})$. Let $\{f_n\} \subset \bigvee(\mathscr{D}_1 \otimes \mathscr{D}_2)$ converge to $f \in \mathscr{D}(\bar{A})$. Then

$$\|\bar{B}(f_n - f_m)\| = \|I_1 \otimes B(f_n - f_m)\| \leqslant a\|I_1 \otimes A_2(f_n - f_m)\| + b\|f_n - f_m\|$$
$$\leqslant a\|A(f_n - f_m)\| + b\|f_n - f_m\| = a\|\bar{A}(f_n - f_m)\| + b\|f_n - f_m\|.$$

Thus $\{\bar{B}f_n\}$ is a Cauchy sequence, and since $\bar{B}$ is closed we have $f \in \mathscr{D}(\bar{B})$ and $\bar{B}f = \lim_{n\to\infty} \bar{B}f_n$, i.e. $\mathscr{D}(\bar{B}) \supset \mathscr{D}(\bar{A})$. A similar estimate gives

$$\|\bar{B}f_n\| \leqslant a\|\bar{A}f_n\| + b\|f_n\| \qquad \text{so that} \qquad \|\bar{B}f\| \leqslant a\|\bar{A}f\| + b\|f\|. \qquad \square$$

*Corollary.* Let $A_i$ and $B$ be as in the lemma. We set $A_2(\lambda) = A_2 + \lambda B$, $|\lambda| < a^{-1}$ and $A(\lambda) = A_1 \otimes I_2 + I_1 \otimes A_2(\lambda)$. Then $\mathscr{D}[\bar{A}(\lambda)]$, the domain of the closure of $A(\lambda)$, is independent of $\lambda$, i.e. equal to $\mathscr{D}(\bar{A})$.

*Proof.* Since $\bar{B}$ is $\bar{A}$-bounded with relative bound $a < 1$ and $\mathscr{D}(\bar{B}) \supset \mathscr{D}(\bar{A})$, it follows that $A'(\lambda) = \bar{A} + \lambda\bar{B}$ is closed on $\mathscr{D}(\bar{A})$. Since $\bar{A}(\lambda)$ and $A'(\lambda)$ are both the closure of $A(\lambda)$, defined on $\bigvee(\mathscr{D}_1 \otimes \mathscr{D}_2)$, they must coincide. Hence $\mathscr{D}[\bar{A}(\lambda)] = \mathscr{D}[A'(\lambda)] = \mathscr{D}(\bar{A})$. $\square$

*Theorem.* The domain $\mathscr{D}(\theta)$ of $\bar{H}_0(\theta)$ is independent of $\theta$, $|\operatorname{Im}\theta| < \pi/4$ and $\{\bar{H}(\theta) \mid |\operatorname{Im}\theta| < \pi/4\}$ is a dilatation analytic family.

*Proof.* We set $H_0(\theta) = \exp(-2\theta)M(\theta) - 1$ where $M(\theta) = T_1 \otimes I_2 + \omega I_1 \otimes [\exp(4\theta)\frac{1}{2}\boldsymbol{x}_2^2 + \frac{1}{2}\boldsymbol{p}_2^2]$ and $M(1) = T_1 \otimes I_2 + I_1 \otimes H^{\text{osc}}$. Since the multiplication operator $\boldsymbol{x}_2^2$ is self-adjoint on $L^2(\mathbb{R}^2)$ with domain strictly larger than $\mathscr{D}(H^{\text{osc}})$, we can apply the above results with $A_1 = T_1$, $A_2 = H^{\text{osc}}$ and $B = \frac{1}{2}\boldsymbol{x}_2^2$. Using the method of § 3, we thus obtain the announced results. $\square$

We now turn to the interaction term $V(\boldsymbol{x}_1 - \rho\boldsymbol{x}_2)$ in (2.11).

*Theorem.* $V(\boldsymbol{x}_1 - \rho\boldsymbol{x}_2)$ is $\bar{H}_0$-bounded with arbitrarily small relative bound and $H$ is self-adjoint on $\mathscr{D}(\bar{H}_0)$.

*Proof.* A standard argument to show that $V$ is relatively bounded with respect to the total kinetic-energy operator on $L^2(\mathbb{R}^5)$ runs as follows. Let $T_2$ be the closure of $-\frac{1}{2}\partial_{x_2}^2$ on $L^2(\mathbb{R}^2)$ and $\bar{T}$ the closure of $T = T_1 \otimes I_2 + I_1 \otimes T_2$. In fact, $\bar{T}$ is the closure of $-\frac{1}{2}\Delta$, $\Delta$ being the Laplacian on $L^2(\mathbb{R}^5)$. Now every $f \in \mathscr{D}(\bar{T})$ is contained in $L^q(\mathbb{R}^5)$, $2 \leqslant q < 10$, (Reed and Simon 1975, theorem 9.28) and $\|f\|_q \leqslant a\|\bar{T}f\| + b\|f\|$ with arbitrarily small $a > 0$. $V$ can be written as $V = V_1 + V_2$ with $V_1 \in L^p(\mathbb{R}^5)$, $1 \leqslant p < 3$ and $V_2 \in L^\infty(\mathbb{R}^5)$. Thus for $f \in \mathscr{D}(\bar{T})$, $\|V_1 f\| \leqslant \|V_1\|_p \|f\|_q$, $p^{-1} + q^{-1} = \frac{1}{2}$, $6 < q < 10$, and

$$\|Vf\| \leqslant a\|V_1\|_p \|\bar{T}f\| + (b\|V_1\|_p + \|V_2\|_\infty)\|f\|. \tag{4.2}$$

In particular, $\mathscr{D}(V) \supset \mathscr{D}(\bar{T})$.

Next we show that $\mathscr{D}(\bar{T}) \supset \mathscr{D}(\bar{H}_0)$. This follows from the inclusion $\mathscr{D}(H^{\text{osc}}) \subset \mathscr{D}(T_2)$ so that $\bigvee \mathscr{D}(T_1) \otimes \mathscr{D}(H^{\text{osc}}) \subset \bigvee \mathscr{D}(T_1) \otimes \mathscr{D}(T_2)$. Now let $\{f_n\} \subset \bigvee \mathscr{D}(T_1) \otimes \mathscr{D}(H^{\text{osc}})$ converge towards $f \in \mathscr{D}(\bar{H}_0)$. Since

$$\begin{aligned}\|T(f_n - f_m)\| &\leqslant \|[\tfrac{1}{2}T_1 \otimes I_2 + (1/\omega) I_1 \otimes H^{\text{osc}} + 1](f_n - f_m)\| \\ &\leqslant (\max\{1, 1/\omega\})\|H_0(f_n - f_m)\| + \|f_n - f_m\|,\end{aligned}$$

it follows that $\{Tf_n\} = \{\bar{T}f_n\}$ is a Cauchy sequence. Consequently $f \in \mathscr{D}(\bar{T})$, i.e. $\mathscr{D}(\bar{H}_0) \subset \mathscr{D}(\bar{T})$, and we also have

$$\|\bar{T}f\| \leqslant (\max\{1, 1/\omega\})\|\bar{H}_0 f\| + \|f\|. \tag{4.3}$$

This, together with (4.2), results in the $\bar{H}_0$-boundedness of $V$ with arbitrarily small relative bound. Since $\mathscr{D}(V) \supset \mathscr{D}(\bar{H}_0)$, this implies the self-adjointness of $H$ on $\mathscr{D} = \mathscr{D}(\bar{H}_0)$. □

*Lemma 2.* The unitary operator $U(\rho) = \exp(\mathrm{i}\rho \boldsymbol{p}_1 \cdot \boldsymbol{x}_2)$, $\rho \in \mathbb{R}$, maps $D = \mathscr{D}(\bar{H}_0)$ onto itself, and $\bar{H}_0(\rho) = U(\rho)\bar{H}_0 U^{-1}(\rho)$ is self-adjoint on $\mathscr{D}$.

*Proof.* There is a set $\mathscr{F} \subset \mathscr{D}$, $\mathscr{F}$ dense in $\mathscr{H}$, such that $U^{-1}(\rho)f \in \mathscr{D}$ for $f \in \mathscr{F}$ and for which (notation $\hat{\boldsymbol{p}}_1 = \{p_{11}, p_{12}, 0\}$)

$$\begin{aligned}H_0(\rho)f \equiv U(\rho)H_0 U^{-1}(\rho)f &= (\bar{H}_0 + \tfrac{1}{2}\rho^2 \omega \hat{\boldsymbol{p}}_1^2 \otimes I_2 + \rho\omega \hat{\boldsymbol{p}}_1 \cdot \boldsymbol{p}_2)f \\ &= (\bar{H}_0 + H_1(\rho))f.\end{aligned}$$

Since $\mathscr{D}(\overline{\hat{\boldsymbol{p}}_1^2 \otimes I_2})$ and $\mathscr{D}(\overline{\hat{\boldsymbol{p}}_1 \cdot \boldsymbol{p}_2})$ contain $\mathscr{D}$, it follows that $H_0(\rho)f$ is defined for every $f \in \mathscr{D}$. Now let $(\lambda, \mu \geqslant 0)$

$$K(\lambda, \mu) = \bar{H}_0 + \tfrac{1}{2}\lambda \hat{\boldsymbol{p}}_1^2 \otimes I_2 + \tfrac{1}{2}\mu I_1 \otimes \boldsymbol{p}_2^2 = \bar{H}_0 + L(\lambda, \mu).$$

By repeated use of relative smallness arguments we find that $K(\lambda, \mu)$ is self-adjoint on $\mathscr{D}$. We now set

$$\overline{H_0(\rho)} = K(\lambda, \mu) + H_1(\rho) - L(\lambda, \mu) = K(\lambda, \mu) + M(\lambda, \mu, \rho).$$

There exist $\lambda_0, \mu_0 \geqslant 0$ such that $M(\lambda_0, \mu_0, \rho) \leqslant aL(\lambda_0, \mu_0)$ for some $a < 1$. But then, since $K(\lambda, \mu) = \bar{H}_0 + L(\lambda, \mu)$, we have for $f \in \mathscr{D}$

$$\|M(\lambda_0, \mu_0, \rho)f\| \leqslant a\|L(\lambda_0, \mu_0)f\| \leqslant a\|K(\lambda_0, \mu_0)f\| + a\omega\|f\|$$

so that $\overline{H_0(\rho)}$ is self-adjoint on $\mathscr{D}$. Now let $\{f_n\} \subset \mathscr{F}$ converge towards $f \in \mathscr{D}$. Then $H_0(\rho)f_n$ converges towards $\overline{H_0(\rho)}f$ and $\bar{H}_0 U^{-1}(\rho)f_n = U^{-1}(\rho)\overline{H_0(\rho)}f_n$ has a limit. Consequently $U^{-1}(\rho)f_n$ converges to an element of $\mathscr{D}$. □

We now turn to the dilated operators $V(\theta)$ and $\tilde{H}_0(\theta)$. For $f \in \mathscr{D}$ and real $\theta$ we have $U(\theta)Vf = V(\theta)U(\theta)f$ with $V(\theta) = \exp(-\theta)V$ (for Coulomb potentials). From now on we shall omit the closure sign over $H_0(\theta)$, $H(\theta)$, etc.

*Proposition.* $V(\theta)$ is $H_0(\theta)$-compact and $K(\theta) = V(\theta)[1+H_0(\theta)]^{-1}$ is compact analytic for $\theta \in \mathbb{C}$ with $|\mathrm{Im}\ \theta| < \pi/4$.

*Proof.* The extension of $V(\theta)$ to complex $\theta$ is well defined for every $f \in \mathscr{D}$, so that $K(\theta)$ is a bounded operator. We now show its compactness. Since $V(\boldsymbol{x}_1 - \rho\boldsymbol{x}_2) = U(-\rho)V(\boldsymbol{x}_1)U(\rho)$, we have ($\frac{1}{2} < \alpha < 1$, $\alpha + \beta = 1$)

$$\begin{aligned} K(\theta) &= \exp(-\theta)U(-\rho)V(\boldsymbol{x}_1)U(\rho)[1+H_0(\theta)]^{-1} \\ &= \exp(-\theta)U(-\rho)V(\boldsymbol{x}_1)(1+\boldsymbol{p}_1^2)^{-\alpha}(1+H^{\mathrm{osc}})^{-\beta} \\ &\quad \times (1+H^{\mathrm{osc}})^{\beta}(1+\boldsymbol{p}_1^2)^{\alpha}(1+H_0)^{-1}(1+H_0)U(\rho)[1+H_0(\theta)]^{-1}. \end{aligned}$$

As $V(\boldsymbol{x}_1)(1+\boldsymbol{p}_1^2)^{-\alpha}$ is compact on $L^2(\mathbb{R}^3)$ and $(1+H^{\mathrm{osc}})^{-\beta}$ is compact on $L^2(\mathbb{R}^2)$, their product is compact on $\mathscr{H}$. Since $(1+H^{\mathrm{osc}})^{\beta} \leqslant (1+H_0)^{\beta}$ and $(1+\boldsymbol{p}_1^2)^{\alpha} \leqslant (1+H_0)^{\alpha}$, it follows that $(1+H^{\mathrm{osc}})^{\beta}(1+\boldsymbol{p}_1^2)^{\alpha}(1+H_0)^{-1}$ is bounded, as is the case for $(1+H_0)U(\rho)[1+H_0(\theta)]^{-1}$ since $U(\rho)$ maps $\mathscr{D}$ onto itself continuously. Thus $K(\theta)$ is the product of a compact operator and bounded operators and consequently is compact. Since $V(\theta)$ is analytic in $\theta$ as a map from $\mathscr{D}$ into $\mathscr{H}$ and $[1+\tilde{H}_0(\theta)]^{-1}$ is analytic in $\theta$, it follows that $K(\theta)$ is compact analytic with analyticity domain $|\mathrm{Im}\ \theta| < \pi/4$. □

*Theorem 3.* $\{H(\theta) = H_0(\theta) + V(\theta) \mid |\mathrm{Im}\ \theta| < \pi/4\}$ is a dilatation analytic family. $\sigma_{\mathrm{ess}}[H(\theta)] = \sigma_{\mathrm{ess}}[H_0(\theta)]$ (the half-lines in figures 1 and 2), $\sigma_{\mathrm{d}}[H(\theta)]$ has as only possible accumulation points the various thresholds $l\omega$, $l = 0, 1, 2, \ldots$ and the points of $\sigma_{\mathrm{d}}[H(\theta)]$ (i.e. the isolated eigenvalues of $H(\theta)$) are independent of $\theta$ (as long as they remain discrete). The singular continuous spectrum of $H = H(0)$ is empty, i.e. $\sigma_{\mathrm{c}}(H) = \sigma_{\mathrm{ac}}(H)$.

*Proof.* Since $V(\theta)$ is $H_0(\theta)$-compact it is $H_0(\theta)$-bounded with arbitrarily small relative bound, so that the dilatation analyticity follows. The invariance of the essential spectrum and the stated properties of $\sigma_{\mathrm{d}}[H(\theta)]$ are further consequences of relative compactness and dilatation analyticity, as is the absolute continuity of the continuous spectrum of $H$ (see Aguilar and Combes 1971, Balslev and Combes 1971). □

In order to learn more about the discrete spectrum of $H(\theta)$, we write it in the form (2.12). Thus

$$H_1(\theta) = H_0(\theta) + V(\boldsymbol{x}_1, \theta) = H^{\mathrm{at}}(\theta) \otimes I_2 + I_1 \otimes H^{\mathrm{osc}}(\theta), \tag{4.4}$$

which is $H(\theta)$ with $\rho = 0$. Theorem 3 still applies, but now we know the exact location of $\sigma_{\mathrm{d}}[H_1(\theta)]$. It consists of eigenvalues $E_{nl} = \epsilon_n + l\omega$, $l = 0, 1, 2, \ldots$, $\epsilon_n$ being an atomic eigenvalue. Since the atomic eigenvalues accumulate at zero, it follows that each threshold $l\omega$ is an accumulation point of $\sigma_{\mathrm{d}}[H_1(\theta)]$. A picture of the situation is given in figure 2. We obtain $H(\theta)$ by perturbing $H_1(\theta)$ with $W(\theta)$:

$$H(\theta) = H_1(\theta) + W(\theta). \tag{4.5}$$

$W(\theta)$ is $H_1(\theta)$-compact since both $V(\boldsymbol{x}_1, \theta)$ and $V(\boldsymbol{x}_1 - \rho\boldsymbol{x}_2, \theta)$ are $H_0(\theta)$-compact and ($E > |\epsilon_0|$)

$$W(\theta)[E+H_1(\theta)]^{-1} = W(\theta)[E+H_0(\theta)]^{-1}[E+H_0(\theta)][E+H_1(\theta)]^{-1},$$

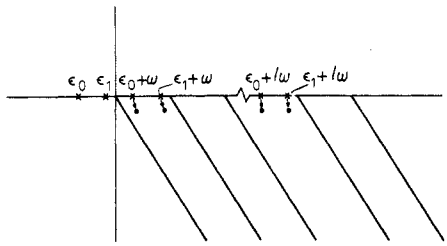


**Figure 2.** The spectrum of $H_1(\theta)$. Crosses are eigenvalues, solid lines continuous spectrum. Note that for $\omega < |\epsilon_n|$, $\epsilon_n + \omega$ is on the negative real axis. Positive eigenvalues are expected to turn into resonances under the perturbation $W$ (indicated by dots).

which is the product of a compact and a bounded operator and hence is compact. Thus $W(\theta)$ will leave the essential spectrum invariant but the discrete spectrum may be changed. In fact, we expect the positive eigenvalues to acquire a negative imaginary part, i.e. to turn into resonances, whereas the negative eigenvalues may be shifted or disappear. We show in the next section that $H(\theta)$ still has an infinite number of negative eigenvalues, which, of course, accumulate at zero.

## 5. The discrete spectrum of $H$ and photoionisation

An H-atom placed in a constant homogeneous electric field does not possess any bound states. In fact the original bound states have turned into resonances. A suitable extension of the dilatation analytic method has recently been applied to this phenomenon (Herbst 1979).

A related problem is the following: what happens to the bound states of an atom when it is placed in a homogeneous sinusoidally oscillating electric field $\boldsymbol{E}(t)$? In the simple case of an electron bound by a (Coulomb) potential $V(\boldsymbol{x})$ and under the influence of such a field, the Hamiltonian is given by ($\boldsymbol{E}(t) = -\partial_t \boldsymbol{A}(t)$)

$$H(t) = \tfrac{1}{2}[\boldsymbol{p} - e\boldsymbol{A}(t)]^2 + V(\boldsymbol{x}), \tag{5.1}$$

which is unitarily equivalent to

$$H^{\mathrm{at}} = \tfrac{1}{2}\boldsymbol{p}^2 + V(\boldsymbol{x}), \tag{5.2}$$

the connecting unitary operator being given by

$$\mathcal{W}(t) = \exp[\mathrm{i}\, e\boldsymbol{A}(t) \cdot \boldsymbol{x}]. \tag{5.3}$$

Thus $H(t)$ possesses bound states, but this result is not relevant to the question whether the time evolution $U(t, t_0)$ associated with $H(t)$ causes the electron to become asymptotically free for a given arbitrarily chosen initial state. An answer to this problem can be obtained by examining the wave operators associated with $U(t, t_0)$ and the corresponding 'free' evolution $U_0(t, t_0)$, the 'free' Hamiltonian being

$$H_0(t) = \tfrac{1}{2}[\boldsymbol{p} - e\boldsymbol{A}(t)]^2. \tag{5.4}$$

The existence proof for the wave operators follows a standard pattern (apart from the modification needed in $U_0(t, t_0)$ to take into account the long-range nature of the Coulomb interaction (Dollard 1964)). If the wave operators are moreover complete,

then we can define the scattering states to be the states in their range $\mathcal{R}$. If $\mathcal{R}$ coincides with the whole Hilbert space $L^2(\mathbb{R}^3)$, then the electron becomes asymptotically free (is ionised) with probability one. If not, then its orthoplement $\mathcal{R}^\perp$ can be said to contain the bound states of the problem.

In an analogous case (Prugovečki and Tip 1974, § 4) it was shown that the wave operators can be defined in terms of the evolution operators associated with the Floquet Hamiltonians (both full and free) of the problem. The same can be done here, so that $\mathcal{R}^\perp$ is precisely the bound-state subspace of the Floquet Hamiltonian $H^{\mathrm{Fl}}$ associated with $U(t, t_0)$. Now $H^{\mathrm{Fl}}$ is believed to be some limiting form of the second quantised Hamiltonian (Shirley 1965, Swain 1973), and within this context we state the main result of this section.

*Theorem 5.1.* The Hamiltonian $H$ given by (2.10) possesses an infinite number of eigenvalues with negative energy. They accumulate at zero.

*Proof.* The idea behind the proof is to show that the negative eigenvalues of $H$ are those of a system consisting of a particle in a potential with an attractive Coulomb tail. In order to do so, we use the Feshbach projection operator formula (see Newton 1966, p 496)

$$(z-H)^{-1} = (z-H_Q)^{-1}Q + [P + (z-H_Q)^{-1}QHP]G_P(z)[P + PHQ(z-H_Q)^{-1}] \tag{5.5}$$

where

$$z \notin \sigma(H), \qquad H_P = PHP, \qquad H_Q = QHQ,$$
$$G_P(z) = [z - H_P - PHQ(z-H_Q)^{-1}QHP]^{-1}. \tag{5.6}$$

The projectors $P$ and $Q = 1 - P$ are defined through $P = I_1 \otimes \hat{P}$, where $\hat{P}$ is the projector upon the ground state of $H^{\mathrm{osc}}$. Since the latter is non-degenerate, $\hat{P}$ is one-dimensional. We start by noting that ($\hat{Q} = I_2 - \hat{P}$; $H_1 = H^{\mathrm{at}} + H^{\mathrm{osc}}$, see (2.13))

$$QH_1Q = H^{\mathrm{at}} \otimes \hat{Q} + I_1 \otimes \hat{Q}H^{\mathrm{osc}}\hat{Q}. \tag{5.7}$$

Its spectrum differs from that of $H_1$ in that $\sigma_{\mathrm{ess}}(QH_1Q)$ starts at $\omega$ instead of zero, since the oscillator ground state is annihilated by $\hat{Q}$. In addition, $QH_1Q$ has discrete eigenvalues $\lambda_n = \epsilon_n + \omega$. In particular, $\omega$ is their accumulation point. (Of course there are also continuum-embedded eigenvalues above $\omega$.) Since $W$ is $H_1$-compact, the same is true for $QWQ$ with respect to $QH_1Q$ on $\mathcal{H}_Q = Q\mathcal{H}$. Thus $\omega$ remains the only possible accumulation point of the discrete spectrum of $H_Q = QH_1Q + QWQ$. In particular, $H_Q$ has only a finite number of eigenvalues (of finite multiplicity) in the interval $(-\infty, \omega - \delta)$, $\delta$ small and positive. We now remove the latter in order to make $PHQ(E-H_Q)^{-1}QHP$ a non-positive operator for $E \leqslant \omega - \delta$. Thus let $\Pi_j$ be the eigenprojector of $H_Q$ corresponding to the eigenvalue $\mu_j \leqslant \omega - \delta$, $j = 1, \ldots, p$, and let $\Pi = \sum_{j=1}^{p} \Pi_j$. Note that $\Pi\mathcal{H} \subset \mathcal{H}_Q$. We now set $\tilde{P} = P + \pi$ and $\tilde{Q} = 1 - \tilde{P}$ and we consider (5.5) and (5.6) with $P$ and $Q$ replaced by $\tilde{P}$ and $\tilde{Q}$, respectively. Then for $z = E$, $E$ real, $E \leqslant \omega - \delta$, $(E - H_Q)^{-1}$ has no singularities, so that the latter, if present, must come from

$$G_{\tilde{P}}(z) = [z - H_{\tilde{P}} - \tilde{P}H\tilde{Q}(z - H_{\tilde{Q}})^{-1}\tilde{Q}H\tilde{P}]^{-1}. \tag{5.8}$$

Now, for $E \leqslant \omega - \delta$,

$$\tilde{P}H\tilde{Q}(E - H_Q)^{-1}\tilde{Q}H\tilde{P} \leqslant 0 \tag{5.9}$$

whereas

$$H_{\tilde{P}} = PHP + \Pi HP + PH\Pi + \Pi H\Pi = H_P + \text{finite rank perturbations.} \tag{5.10}$$

The spectrum of $H_P$ is that of

$$H_{\text{eff}} = \tfrac{1}{2}\boldsymbol{p}_1^2 + V_{\text{eff}}(\boldsymbol{x}_1) \tag{5.11}$$

on $L^2(\mathbb{R}^3)$, where

$$\begin{aligned} V_{\text{eff}}(\boldsymbol{x}_1) &= \int \mathrm{d}\boldsymbol{x}_2\ V(\boldsymbol{x}_1 - \rho\boldsymbol{x}_2)|u_0(\boldsymbol{x}_2)|^2 \\ &= -(Z/\pi)\int \mathrm{d}\boldsymbol{x}_2\,(\boldsymbol{x}_1 - \rho\boldsymbol{x}_2)^{-1}\exp(-\boldsymbol{x}_2^2). \end{aligned} \tag{5.12}$$

This potential has an attractive Coulomb tail, and consequently has an infinite set of negative eigenvalues accumulating at zero. This behaviour is not changed by the finite-rank perturbations in (5.10), whereas the non-positive operator (5.9) can only lower their values. In principle, this operator can shift the accumulation point, but we know already that the lowest accumulation point of $\sigma_{\text{d}}(H)$ is zero. Thus we find that $G_{\tilde{P}}(z)$, and hence $(z-H)^{-1}$, has an infinite number of negative poles of finite multiplicity, accumulating at zero. Consequently the same is true for the negative eigenvalues of $H$.

Since $H$ possesses bound states, it will be evident that a system which is in some state $\Psi(0)$ at time $t=0$ need not be ionised with probability one as $t$ tends to infinity. This clearly depends on whether $\Psi(0)$ contains bound-state contributions. On the other hand, it is sometimes believed that the ionisation probability tends to one as the field intensity (i.e. the number of photons in the initial state) increases. We shall now prove a result in this direction. Let $\Psi(0)$ be of the form

$$\Psi(0) = v_n \times u_l = \Psi_{nl} \tag{5.13}$$

where $v_n$ is an eigenstate of $H^{\text{at}}$ with eigenvalue $\epsilon_n$ and $u_l$ an eigenstate of $H^{\text{osc}}$ with eigenvalue $l\omega$. Then, as $l$ increases, $\Psi(0)$ becomes orthogonal to each eigenstate of $H$ with eigenvalue smaller than some real constant $\Lambda$.

*Theorem 5.2.* Let $P$ be the projector upon the bound-state subspace of $\mathcal{H}$ spanned by the eigenvectors $\phi_j$ of $H$ with eigenvalues $\lambda_j$ smaller than $\Lambda$. Then $P\Psi_{nl}$ tends to zero in norm as $l$ tends to infinity.

*Proof.* We take $l$ so large that the eigenvalue $E_{nl} = \epsilon_n + l\omega$ of $H_1$ is larger than $\Lambda$. Since

$$(H\phi_j, \Psi_{nl}) = \lambda_j(\phi_j, \Psi_{nl}) = (\phi_j, H\Psi_{nl}) = E_{nl}(\phi_j, \Psi_{nl}) + (W\phi_j, \Psi_{nl}), \tag{5.14}$$

we have

$$\begin{aligned} \|P\Psi_{nl}\|^2 &= \sum_j |(\phi_j, \Psi_{nl})|^2 = \sum_j (E_{nl} - \lambda_j)^{-2}|(W\phi_j, \Psi_{nl})|^2 \\ &\leqslant (E_{nl} - \Lambda)^{-2}\sum_j |(\phi_j, W\Psi_{nl})|^2 \\ &= (E_{nl} - \Lambda)^{-2}\|PW\Psi_{nl}\|^2 \leqslant (E_{nl} - \Lambda)^{-2}\|W\Psi_{nl}\|^2. \end{aligned}$$

Now, since $v_n(x_1)$, and hence $|v_n(x_1)|^2$, is an element of $L^\infty(\mathbb{R}^3)$,

$$\begin{aligned}
\|W\Psi_{nl}\|^2 &= \int \mathrm{d}x_1\,\mathrm{d}x_2(|x_1-\rho x_2|^{-1}-|x_1|^{-1})^2|v_n(x_1)|^2|u_l(x_2)|^2 \\
&\leqslant \|v_n^2\|_\infty \int \mathrm{d}x_2\,\mathrm{d}x_1(|x_1-\rho x_2|^{-1}-|x_1|^{-1})^2|u_l(x_2)|^2 \\
&\leqslant 4\pi\rho\|v_n^2\|_\infty \int \mathrm{d}x_2\,|x_2||u_l(x_2)|^2 \\
&\leqslant 4\pi\rho\|v_n^2\|_\infty \int \mathrm{d}x_2\,(1+|x_2|^2)|u_l(x_2)|^2 \\
&= 4\pi\rho\|v_n^2\|_\infty\Big(1+\int_{-\infty}^{+\infty}\mathrm{d}w\,w^2(|u_{l_1}(w)|^2+|u_{l_2}(w)|^2)\Big) \\
&= 4\pi\rho\|v_n^2\|_\infty[1+\tfrac{1}{2}(l_1+1)+\tfrac{1}{2}l_1+\tfrac{1}{2}(l_2+1)+\tfrac{1}{2}l_2] \\
&= 4\pi\rho\|v_n^2\|_\infty[2+\tfrac{1}{2}(l_1+l_2)] = K(2+\tfrac{1}{2}l),
\end{aligned}$$

where we have used the well known recursion relations for Hermite functions. Thus

$$\|P\Psi_{nl}\|^2 \leqslant (\epsilon_n + l\omega - \Lambda)^{-2}K(2+\tfrac{1}{2}l)$$

and the right-hand side tends to zero with increasing $l$. □

This result is still not completely satisfactory, since there may be bound states of $H$ with arbitrarily large energy. On the other hand, we expect the corresponding states of $H$ to turn into resonances under the perturbation $W$, so that only negative-energy bound states would remain. The situation here is similar to the one encountered in dealing with autoionising atomic states (although there positive-energy bound states or resonances do not occur (see Simon 1972)). In fact the analysis given by Simon (1973) applies here as well. In particular, this is the case for his derivation of the 'Golden Rule' expression for the imaginary part of the leading term in a perturbation expansion of complex eigenvalues.

## 6. Discussion and outlook

### *6.1. Dilatations and resonances*

In § 2 we made a formal unitary transformation in order to bring the Hamiltonian into a form where relative compactness properties of the interaction $W$ could be used. In fact, this unitary transformation was given a precise meaning by lemma 2 of § 4. It is important to note that the unitary operator $U(\lambda) = \exp(\mathrm{i}\lambda \boldsymbol{p}_1 \cdot \boldsymbol{x}_2)$, implementing this transformation, is invariant under dilatations. This property is quite important, since unitarily equivalent Hamiltonians may have different spectra upon complex dilatation. An example is the following. Consider a particle in an attractive potential with no bound states, and suppose that the wave operators exist and are unitary. Then the full Hamiltonian is unitarily equivalent to the kinetic energy operator. Now the former may, upon complex dilatation, have complex eigenvalues but the latter does not.

A second possible dilatation transformation would be to dilate only the electronic position and momentum operators but not those of the oscillator. This cannot be done with the Hamiltonian (2.10), since the potential is not analytic under such transformations (also $U(\lambda)$ becomes unbounded). The situation is different for the Hamiltonian (2.7). If we scale away the factor $\omega$, we have a zero-order Hamiltonian of the form

$$H_\alpha(\theta) = \tfrac{1}{2}\boldsymbol{p}_1^2 \exp(-2\theta) \otimes I_2 + I_1 \otimes [\tfrac{1}{2}(\boldsymbol{p}_2^2 + \boldsymbol{x}_2^2) - 1]. \tag{6.1}$$

Again, sectoriality properties can be used to obtain its spectrum for complex $\theta$ (the by now familiar set of half-lines). The potential $V(\boldsymbol{x}_1, \theta) = \exp(-\theta)V(\boldsymbol{x}_1)$ is $H_\alpha(\theta)$-compact and causes no problems, so that only the perturbation

$$H_\beta(\theta) = -\exp(-\theta)\lambda \boldsymbol{p}_1 \cdot \boldsymbol{p}_2, \qquad \lambda = \sigma/(\sigma^2 + \tilde{\omega}), \tag{6.2}$$

remains to be considered.

*Proposition.* $H_\beta(\theta)$ is $H_\alpha(\theta)$-bounded with relative bound smaller than one.

*Proof.* We omit the $-1$ in the oscillator Hamiltonian for notational convenience. Then, writing

$$\exp(\theta) = \rho \exp(\mathrm{i}\psi), \qquad \exp(-2\theta) = a + \mathrm{i}b, \qquad a = \rho^{-2}\cos 2\psi,$$
$$b = \rho^{-2}\sin 2\psi,$$

we have for $f \in \mathcal{D}[H_\alpha(\theta)]$

$$\|H_\alpha(\theta)f\|^2 = \|[\tfrac{1}{2}a\boldsymbol{p}_1^2 + \tfrac{1}{2}(\boldsymbol{p}_2^2 + \boldsymbol{x}_2^2)]f\|^2 + \|\tfrac{1}{2}b\boldsymbol{p}_1^2 f\|^2.$$

Since

$$\pm \boldsymbol{p}_1 \cdot \boldsymbol{p}_2 \leqslant \tfrac{1}{2}(\mu \boldsymbol{p}_1^2 + \mu^{-1}\boldsymbol{p}_2^2), \qquad \mu > 0,$$

we have ($\sigma, \tau \geqslant 0$, $\sigma + \tau = 1$)

$$\begin{aligned}\|H_\beta(\theta)f\|^2 &\leqslant (\lambda/\rho)\|(\tfrac{1}{2}\mu\boldsymbol{p}_1^2 + \tfrac{1}{2}\mu^{-1}\boldsymbol{p}_2^2)f\| \\ &\leqslant (\lambda/\rho)[(\mu\sigma/|a|)\|\tfrac{1}{2}a\boldsymbol{p}_1^2 f\| + (\mu\tau/|b|)\|\tfrac{1}{2}b\boldsymbol{p}_1^2 f\| + \mu^{-1}\|\tfrac{1}{2}\boldsymbol{p}_2^2 f\|] \\ &\leqslant (\lambda/\rho)(\mu\sigma/|a| + \mu\tau/|b| + \mu^{-1})\|H_\alpha(\theta)f\|^2.\end{aligned}$$

Taking $\sigma = \cos^2 2\psi$, $\tau = \sin^2 2\psi$ and $\mu = \rho^{-1}$, we obtain

$$\begin{aligned}\|H_\beta(\theta)f\|^2 &\leqslant (\lambda/\rho)(\mu\rho^2|\cos 2\psi| + \mu\rho^2|\sin 2\psi| + \mu^{-1})\|H_\alpha(\theta)f\|^2 \\ &\leqslant 3\lambda\|H_\alpha(\theta)f\|^2.\end{aligned}$$

Since $\lambda < \frac{1}{3}$ (see § 2), we have obtained the announced result for $a$, $b$ both non-zero, the case that one of the two vanishes being even simpler.

According to this result $\{H(\theta) = H_\alpha(\theta) + H_\beta(\theta) + V(\theta) | \theta \in \mathbb{C}\}$ is a dilatation analytic family. It must however be remembered that, since $H_\beta(\theta)$ is not relatively compact, the essential spectrum is in general not invariant under the perturbation $H_\beta(\theta)$ (this is already the case for real $\theta$).

We note further that the above type of estimate shows that it is possible to make an analytic continuation in the coupling constant $\lambda$.

*6.2. Applications to photoionisation and scattering processes*

In expressions related to photoionisation probabilities and scattering amplitudes, matrix elements of the resolvent $(z-H)^{-1}$, $z=E+\mathrm{i}\epsilon$, $E$ real, appear:

$$\Phi(z)=([z-H]^{-1}f,\, g)=([z-H(\theta)]^{-1}U(\theta)f,\, U(\theta)g). \tag{6.3}$$

Here $U(\theta)$ is a unitary operator of the dilatation group. If the states $f(\theta)=U(\theta)f$ and $g(\theta)=U(\theta)g$ can be continued analytically for complex $\theta$, then we can continue $\Phi(z)$ into the lower half plane and it becomes possible to disentangle pole contributions close to the energy $E$ from the complex dilated resolvent.

Thus, if we can calculate the corresponding complex eigenvalue and eigenfunction of $H(\theta)$ with some degree of accuracy, then a pole approximation to the resolvent can be expected to give a reasonable approximation to the resonant structure of $\Phi(z)$ for energy $E$ near the pole. In a future publication we intend to discuss resonant two-photon ionisation processes in this manner.

Another, even more fundamental, aspect of ionisation and scattering processes is the existence and completeness of the wave operators. We mention, without giving the (straightforward) proof, that the wave operators associated with the full Hamiltonian $H$ and the channel Hamiltonian $H_0$ (see § 2) indeed exist. The only complication is the use of a modified free evolution operator as first given by Dollard (1964), which is necessary due to the long-range nature of the Coulomb interaction. We did not investigate the completeness property but it seems that a suitable modification of Enss's method (Enss 1978a, b) should work.

*6.3. Many-electron systems and resonance spectroscopy*

The equivalent of the Hamiltonian (2.10) for a system consisting of $N$ electrons and an infinitely heavy nucleus with charge $Z$ is

$$H=H^{\mathrm{at}}+H^{\mathrm{osc}}+W=H_1+W \tag{6.4}$$

where now, using the index 0 for oscillator variables,

$$H^{\mathrm{at}}=\sum_{j=1}^{N}\tfrac{1}{2}\boldsymbol{p}_j^2+\sum_{1\leqslant i<j\leqslant N}|\boldsymbol{x}_i-\boldsymbol{x}_j|^{-1}-\sum_{j=1}^{N}Z|\boldsymbol{x}_j|^{-1}, \tag{6.5}$$

$$H^{\mathrm{osc}}=\omega[\tfrac{1}{2}(\boldsymbol{p}_0^2+\boldsymbol{x}_0^2)-1] \tag{6.6}$$

and

$$W=Z\sum_{j=1}^{N}(|\boldsymbol{x}_j|^{-1}-|\boldsymbol{x}_j-\rho\boldsymbol{x}_0|^{-1}). \tag{6.7}$$

We plan to give a full discussion of the dilatation analytic properties of this system on another occasion, but here we want to mention an interesting phenomenon that does not occur in the one-electron case. The point is that now $H^{\mathrm{at}}$, upon complex dilatation, possesses complex eigenvalues $\epsilon_n$, the atomic resonances. We can imagine the situation that the eigenvalue $\epsilon_n+\omega$ of $H_0$ is close to a second resonance eigenvalue $\epsilon_m$. Then $W$ will cause a relatively strong coupling between the states corresponding to these complex energy eigenvalues. Recent experiments (Langendam and van der Wiel 1978) confirm this idea. The experimental set-up is such that an atomic system ($e^-+Ne$) in a state $n(\epsilon_n)$ is brought to a state $m(\epsilon_m)$ by absorption of a photon. A resonance structure is then observed when the photon frequency matches the difference in the real parts of

the energies $\epsilon_n$ and $\epsilon_m$. By making a suitable pole approximation to the resolvent $[z-H(\theta)]^{-1}$, it is possible to obtain a reasonable description of this resonance behaviour (A Tip, work in progress).

## Acknowledgments

AT was supported by the Foundation for Fundamental Research on Matter (FOM) which is sponsored by the Netherlands Organization for the Advancement of Pure Research (ZWO).

The authors are indebted to J M Combes for useful discussions, especially in connection with theorem 5.1.

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