Hydrogen atom in the four-dimensional oscillator representation: matrix elements of z^n

1985 J. Phys. A: Math. Gen. 18 2719

(http://iopscience.iop.org/0305-4470/18/14/022)

J. Phys. A: Math. Gen. **18** (1985) 2719-2727. Printed in Great Britain

Hydrogen atom in the four-dimensional oscillator representation: matrix elements of z^n†

Hilda A Cerdeira‡

Serin Physics Laboratory, Rutgers University, Piscataway, NJ 08854, USA

Received 15 January 1985

Abstract. We present a calculation of the matrix elements of z^n between four-dimensional harmonic oscillator states. We show that a knowledge of the scalar product of two harmonic oscillator states of different frequencies is enough to generate the matrix elements of any power of z. These can be found by taking appropriate derivatives of the aforementioned scalar product.

1. Introduction

Experiments performed by Bayfield *et al* (1977) on hydrogen atoms in an oscillating electric field showed that resonant multiphoton transitions can be stimulated. This in turn enhances the atomic ionisation rate. These stochastic processes (Leopold and Percival 1979) cannot be explained by direct tunnelling, even considering the effects of crossing of Stark energy levels (Littman *et al* 1976). This is the first experimental evidence for chaotic behaviour in a quantum dynamical system. It is, therefore, important to obtain an adequate theoretical description of this problem. The three-dimensionality of the system, however, poses formidable mathematical difficulties. Some authors (Blümel and Smilansky 1984, Jensen 1982, 1984) studied analogous systems represented by a one-dimensional hydrogen atom. They found stochastic ionisation only in the classical limit, while chaos is suppressed in the quantum mechanical treatment. This simplified model is clearly inadequate to explain the experiments described above (Bayfield *et al* 1977). In order to accomplish this, exact solutions for the three-dimensional quantum problem are needed. The first step in this direction consists of calculating the matrix elements of z, and of any power of z, between quantum states of different energies. With these matrix elements the problem of ionisation of hydrogen atoms can be solved to any degree of accuracy using quantum maps (Hogg and Huberman 1983, Zavslavsky 1981).

As the calculation of those matrices between states in the $|Nlm\rangle$ representation becomes very difficult, we suggest solving the problem in the four-dimensional oscillator representation. We make use of the fact that a three-dimensional hydrogen atom is equivalent to a four-dimensional harmonic oscillator with constraints (Boiteux 1973, Kibler and Négadi 1983a, b, 1984). In this spirit it is possible to write the Hamiltonian as that of a set of coupled oscillators with time dependent coupling constants, which, later on, can be handled by different methods. In this representation the matrix elements

† Supported in part by the National Science Foundation under Grant No DMR-82-16223.

‡ Permanent address: Instituto de Fisica, UNICAMP, 13100, Campinas, SP, Brazil.

0305-4470/85/142719+09$02.25

of the perturbation can be calculated between states of different n (the main quantum number of the hydrogen atom). The aim of this paper is to give explicit analytic expressions for those matrix elements and show how to generate matrix elements of higher powers of z.

The remainder of this paper is organised as follows: in § 2 we present the four-dimensional representation of the hydrogen atom. In § 3 we calculate the matrix elements of z. In § 4 we present a discussion on approaches to the solution of the time dependent Schrödinger equation. Finally, we summarise the work in § 5.

2. Four-dimensional representation of the hydrogen atom

Consider a hydrogen atom in three dimensions, in the presence of an electric field $E(t)$. The Hamiltonian is given by

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{r} + eE(t)z$$
$$= H_0 + eE(t)z, \tag{2.1}$$

where μ is the reduced mass of the hydrogen atom and e the charge of the electron. The equivalent problem in four dimensions is found using the Kustaanheimo-Stiefel (KS) transformation of the configuration space (Boiteux 1973):

$$\begin{pmatrix} \boldsymbol{r} \\ 0 \end{pmatrix} = A(u)\boldsymbol{u}, \tag{2.2}$$

where

$$A(u) = \begin{pmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix}, \tag{2.3}$$

$$r = \sum_{\alpha=1}^{4} u_\alpha^2, \tag{2.4}$$

subject to the restriction:

$$R|\Psi\rangle = (u_1 v_4 - u_4 v_1 + u_3 v_2 - u_2 v_3)|\Psi\rangle = 0, \tag{2.5}$$

which is necessary for the eigenfunction to be single-valued (Boiteux 1973, Kibler and Négadi 1984). In order for the transformation to be canonical, the momenta must transform as

$$\begin{pmatrix} \boldsymbol{p} \\ (1/2r)R \end{pmatrix} = (1/2r)A(u)\boldsymbol{v}. \tag{2.6}$$

Under the KS transformation, the Schrödinger equation for the unperturbed hydrogen atom can be written as (Boiteux 1973, 1982, Chen 1980, Kibler and Négadi 1984, Landau 1958):

$$\left(-\frac{\hbar^2}{2\mu} \sum_{\alpha=1}^{4} \frac{\partial^2}{\partial u_\alpha^2} - 4E \sum_{\alpha=1}^{4} u_\alpha^2 - 4e^2 \right) \Psi = 0. \tag{2.7}$$

Equation (2.7) is the Schrödinger equation of a four-dimensional harmonic oscillator, whose solution is given by

$$\Psi_{n,n_1,n_2,n_3,n_4}(u_1, u_2, u_3, u_4) = \prod_{i=1}^{4} \Phi_{n,n_i}(u_i), \tag{2.8}$$

with

$$\Phi_{n,n_i}(u_i) = C_{n,n_i} \exp[-(\mu/2\hbar)\omega_n u_i^2] H_{n_i}((\mu\omega_n/\hbar)^{1/2} u_i). \tag{2.9}$$

Here C_{n,n_i} is a normalisation constant and $H_n(x)$ is a Hermite polynomial. The frequencies, ω_n, of the harmonic oscillators represented by (2.8) and (2.9) are related to the energy eigenvalues, E_n, of the hydrogen atom by

$$\tfrac{1}{2}\mu\omega_n^2 = -4E_n, \tag{2.10}$$

with

$$E_n = -(e^4\mu/2\hbar^2)/n^2, \tag{2.11}$$

and

$$n_1 + n_2 + n_3 + n_4 + 2 = 2n. \tag{2.12}$$

Here, n_i is the ith quantum number of the four-dimensional harmonic oscillator. Equation (2.12) is a consequence from the invariance $\Psi(u) = \Psi(-u)$ (Boiteux 1973). The constraint given by equation (2.5) was shown by Boiteaux (1982) to restrict the degeneracy of the corresponding eigenstates of the four-dimensional harmonic oscillator, to match the accidental degeneracy of the corresponding levels of the hydrogen atom. It is important to notice that the functions given by (2.8) and (2.9) do not form an orthogonal basis. This peculiarity introduces coupling between the eigenmodes even in the absence of an external perturbation (Kibler and Négadi 1984, Chen 1982), and is a direct consequence of the constraint given by (2.10).

3. The matrix elements

3.1. The scaling operator

We denote the basis functions of (2.8) by

$$|n, \{n_i\}\rangle = \prod_{i=1}^{4} |n, n_i\rangle, \tag{3.1}$$

where

$$|n, n_i\rangle = \Phi_{n,n_i}(u_i), \tag{3.2}$$

with $\Phi_{n,n_i}(u)$ given by (2.9). In order to calculate the matrix elements we define a scaling operator $S(\beta)$ in one dimension, as (Englefield 1972):

$$f(\beta x) = \beta^{-1/2} S(\beta) f(x), \qquad \text{for } \beta > 0 \tag{3.3}$$

therefore

$$|n, n_i\rangle = (\omega_n/\omega_0)^{-1/4} S((\omega_n/\omega_0)^{1/2}) |1, n_i\rangle \tag{3.4}$$

where the scaling operator has the form:

$$S(\beta) = \exp[(\tfrac{1}{2} + x\,\partial/\partial x)\log\beta], \tag{3.5}$$

and $\omega_n = \omega_0/n$, with $\omega_0 = 2e^2/\hbar$.

Let us start with the matrix element of z, which in the four-dimensional representation is given by $32\langle n, \{n_i\}|u^2(u_1u_3 + u_2u_4)|m, \{m_i\}\rangle$, to show how the method works. The extra term $16u^2 \equiv 16(u_1^2 + u_2^2 + u_3^2 + u_4^2)$ comes from the volume element in four-dimensional space, which we have to include since we are *not* incorporating it in our definition of the scalar products (see (3.11)). Since the wavefunction is separable in the u_i variable, we only need to calculate matrix elements like $\langle n, n_i|u_i^k|m, m_i\rangle$, with $k = 0, 1, 2$ and 3. In § 3.3 we show that the knowledge of $\langle n, n_i|u_i^k|m, m_i\rangle$ for $k = 0$ and 1 is enough to generate all powers. Let us start with $k = 1$. Using (3.4) we have

$$\langle n, n_i|u|m, m_i\rangle = (nm)^{1/4}\langle 1, n_i|S^+((\omega_n/\omega_0)^{1/2})uS((\omega_m/\omega_0)^{1/2})|1, m_i\rangle. \tag{3.6}$$

It is easy to see that

$$S(\beta)u = \beta uS(\beta)$$

$$S^+(\beta^{-1}) = S(\beta)$$

and

$$S(\alpha)S(\beta) = S(\alpha\beta).$$

Therefore, (3.6) becomes

$$\langle n, n_i|u|m, m_i\rangle = (nm)^{1/4}m^{1/2}\langle 1, n_i|S((n/m)^{1/2})u|1, m_i\rangle. \tag{3.7}$$

Since the functions $|1, n_i\rangle$ form a complete set, (3.7) can be written as

$$\langle n, n_i|u|m, m_i\rangle = (mn)^{-1/4}\sum_l \langle 1, n_i|S((n/m)^{1/2})|1, l\rangle\langle 1, l|u|1, m_i\rangle \tag{3.8}$$

which becomes:

$$\begin{aligned}\langle n, n_i|u|m, m_i\rangle &= (nm)^{1/4}(\hbar/\mu\omega_m)^{1/2}\{(\tfrac{1}{2}m_i)^{1/2}\langle 1, n_i|S((n/m)^{1/2})|1, m_i - 1\rangle \\ &\quad + [\tfrac{1}{2}(m_i + 1)]^{1/2}\langle 1, n_i|S((n/m)^{1/2})|1, m_i + 1\rangle\}.\end{aligned} \tag{3.9}$$

We notice that the problem reduces to calculation of $\langle 1, n_i|S((n/m)^{1/2})|1, m_i\rangle$, which is equal to $\langle n, n_i|m, m_i\rangle$. We devote § 3.2 to the evaluation of these functions.

3.2. Calculation of the basic matrix elements

Let us define

$$S_{n,m}^{n_i,m_i} = \langle 1, n_i|S((n/m)^{1/2})|1, m_i\rangle \tag{3.10}$$

or:

$$\begin{aligned}S_{n,m}^{n_i,m_i} = C_{n,n_i}^* C_{m,m_i}\int_{-\infty}^{\infty} du\,\exp[-(\mu/2\hbar)(\omega_n + \omega_m)u^2] \\ \times H_{n_i}((\mu\omega_n/\hbar)^{1/2}u)H_{m_i}((\mu\omega_m/\hbar)^{1/2}u),\end{aligned} \tag{3.11}$$

where

$$C_{n,n_i} = 2^{-n_i/2}(n_i!)^{-1/2}(\mu\omega_n/\pi\hbar)^{1/4}.$$

To calculate the integral in (3.11) we make use of the following relations (Gradshteyn and Ryzhik 1980):

$$H_{2n}(x) = (-1)^n 2^{2n} n!\, L_n^{-1/2}(x^2) \tag{3.12a}$$

$$H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x L_n^{1/2}(x^2), \tag{3.12b}$$

where the $L_n^{\alpha}(x)$ are the associated Laguerre polynomials. It is clear from (3.11) that

$$S_{n,m}^{n_i,m_i} = 0 \tag{3.13}$$

when n_i and m_i have different parity, independent of n and m, since the integrand will be an odd function. Let us consider two cases: when n_i and m_i are even, and when they are odd.

3.2.1. n_i and m_i even. After substitution of (3.12*a*) into (3.11), and change of variables, $S_{n,m}^{n_i,m_i}$ can be written as:

$$S_{n,m}^{n_i,m_i} = \frac{(-2)^{(n_i+m_i)/2}}{(n_i!m_i!)^{1/2}} \left(\frac{\mu\omega_n}{\pi\hbar}\right)^{1/4} \left(\frac{\mu\omega_m}{\pi\hbar}\right)^{1/4} \left(\frac{n_i}{2}\right)! \left(\frac{m_i}{2}\right)! \times \int_{-\infty}^{\infty} dx \exp(-(\mu/2\hbar)(\omega_n+\omega_m)x) x^{-1/2} L_{n_i/2}^{-1/2}\left(\frac{\mu\omega_n}{\hbar}x\right) L_{m_i/2}^{-1/2}\left(\frac{\mu\omega_m}{\hbar}x\right). \tag{3.14}$$

Therefore, we find for the basic matrix element $S_{n,m}^{n_i,m_i}$ (Gradshteyn and Ryzhik 1980):

$$S_{n,m}^{n_i,m_i} = \frac{(-)^{m_i/2} 2^{(n_i+m_i)/2}}{(n_i!m_i!)^{1/2}} \left(\frac{2}{\pi}\right)^{1/2} \frac{(nm)^{1/4}}{(n+m)^{1/2}} \left(\frac{m-n}{m+n}\right)^{(n_i+m_i)/2} \times \Gamma(\tfrac{1}{2}(n_i+m_i+1)) F\left(-\frac{m_i}{2}, -\frac{n_i}{2}; -\frac{(m_i+n_i)}{2}+\frac{1}{2}; \left(\frac{m+n}{m-n}\right)^2\right), \tag{3.15}$$

where $F(\alpha, \beta; \gamma; z)$ is the hypergeometric function, which in this case reduces to a polynomial, since α and β are negative integers. In (3.15) the Gamma function is defined by:

$$\Gamma(n+\tfrac{1}{2}) = (2n-1)!!\pi^{1/2}/2^n.$$

In the limit $n \to m$, the matrix elements of (3.15) are the scalar products of two harmonic oscillator eigenstates of the same frequency. Hence it must have the limiting value

$$\lim_{n\to m} S_{n,m}^{n_i,m_i} = \delta_{n_i,m_i}.$$

It is straightforward, though tedious, to verify that (3.15) satisfies this condition.

3.2.2. n_i and m_i odd. Following the same steps as before, but using (3.12*b*) for the Hermite polynomials, it is easy to find for the basic matrix elements:

$$S_{n,m}^{n_i,m_i} = \frac{(-)^{(m_i-1)/2} 2^{(n_i+m_i)/2}}{(n_i!\,m_i!)^{1/2}} \frac{(nm)^{3/4}}{(m+n)^{3/2}} \frac{2^{3/2}}{\pi^{1/2}} \left(\frac{m-n}{m+n}\right)^{(m_i+n_i)/2-1} \times \Gamma\left(\frac{m_i+n_i+1}{2}\right) F\left(-\frac{m_i-1}{2}, -\frac{n_i-1}{2}; -\frac{m_i+n_i}{2}+\frac{1}{2}; \left(\frac{m+n}{m-n}\right)^2\right) \tag{3.16}$$

which again reduces to δ_{n_i,m_i}, when $n \to m$.

In terms of the calculated matrix elements, the matrix element of $z = 2(u_1u_3 + u_2u_4)$, mentioned in § 3.1, have the form:

$$\langle n, \{n_i\}|z|m, \{m_i\}\rangle$$

$$\begin{aligned}
&= 8(nm)^{1/4}(\hbar/\mu\omega_m)^{3/2}\Big\{ S^{n_2,m_2}_{n,m} S^{n_4,m_4}_{n,m}[(m_1^{1/2}\, S^{n_1,m_1-1}_{n,m} + (m_1+1)^{1/2} S^{n_1,m_1+1}_{n,m}) \\
&\quad \times([m_3(m_3-1)(m_3-2)]^{1/2} S^{n_3,m_3-3}_{n,m} + 3m_3^{3/2} S^{n_3,m_3-1}_{n,m} \\
&\quad + 3(m_3+1)^{3/2} S^{n_3,m_3+1}_{n,m} + [(m_3+1)(m_3+2)(m_3+3)]^{1/2} S^{n_3,m_3+3}_{n,m}) + ① \leftrightarrow ③] \\
&\quad + (m_2^{1/2} S^{n_2,m_2-1}_{n,m} + (m_2+1)^{1/2} S^{n_2,m_2+1}_{n,m})(m_4^{1/2} S^{n_4,m_4-1}_{n,m} + (m_4+1)^{1/2} S^{n_4,m_4+1}_{n,m}) \\
&\quad \times[S^{n_3,m_3}_{n,m}([m_2(m_2-1)]^{1/2} S^{n_2,m_2-2}_{n,m} + (2m_2+1) S^{n_2,m_2}_{n,m} \\
&\quad + [(m_2+1)(m_2+2)]^{1/2} S^{n_2,m_2+2}_{n,m}) + ② \leftrightarrow ④] + \begin{bmatrix} ① \leftrightarrow ② \\ ③ \leftrightarrow ④ \end{bmatrix} \Big\}
\end{aligned} \tag{3.17}$$

where $+(i) \leftrightarrow (j)$ means to add a term like the previous one within the parentheses with i and j permuted. It is understood that $S^{n_i,m_i}_{n,m}$ should be made equal to zero whenever n_i or m_i becomes negative. Using the constraints on the four-dimensional harmonic oscillator, given by (2.12), it is easy to convince oneself that there are eight equivalent terms to (3.17), when we consider all the permutations of the n_i's.

3.3. Generation of matrix elements of the form $\langle n, n_i|u^k|m, m_i\rangle$

In order to calculate the matrix elements of any power of z, it suffices to calculate matrix elements like $\langle n, n_i|u_i^k|m, m_i\rangle$, $k = 0, 1, 2, 3, \ldots$. It is easy to see that we can generate those matrix elements from the knowledge of $S^{n_i,m_i}_{n,m}$ of a new variable. Let us define:

$$\begin{aligned}
S^{n_i,m_i}_{n,m}(y) &= C^*_{n,n_i} C_{m,m_i} \int_{-\infty}^{\infty} \mathrm{d}u \exp[-y(\mu/2\hbar)(\omega_n + \omega_m)u^2] \\
&\quad \times H_{n_i}((\mu\omega_n/\hbar)^{1/2}u) H_{m_i}((\mu\omega_m/\hbar)^{1/2}u),
\end{aligned} \tag{3.18}$$

where

$$S^{n_i,m_i}_{n,m} = S^{n_i,m_i}_{n,m}(1).$$

It is straightforward to see that:

$$\langle n, n_i|u^{2l}|m, m_i\rangle = \left(-\frac{2\hbar mn}{\mu\omega_0(m+n)}\right)^l \frac{\partial^l}{\partial y^l} S^{n_i,m_i}_{n,m}(y)|_{y=1}. \tag{3.19}$$

While the odd powers are generated by:

$$\langle n, n_i|u^{2l+1}|m, m_i\rangle = \left(-\frac{2\hbar}{\mu\omega_0}\frac{mn}{(m+n)}\right)^l \frac{\partial^l}{\partial y^l}\langle n, n_i|u|m, m_i\rangle_y|_{y=1} \tag{3.20}$$

where, in analogy with (3.9):

$$\begin{aligned}
&\langle n, n_i|u|m, m_i\rangle_y \\
&\quad = (nm)^{-1/4}(\hbar/\mu\omega_0)^{1/2}\left\{\left(\frac{m_i}{2}\right)^{1/2} S^{n_i,m_i-1}_{n,m}(y) + \left(\frac{m_i+1}{2}\right)^{1/2} S^{n_i,m_i+1}_{n,m}(y)\right\}.
\end{aligned} \tag{3.21}$$

An expression for $S^{n_i,m_i}_{n,m}(y)$ is easily calculated in the way described in § 3.2, and we find the following.

(a) When n_i and m_i have different parity, independent of n and m

$$S^{n_i,m_i}_{n,m}(y)=0.$$

(b) When n_i and m_i are even

$$S^{n_i,m_i}_{n,m}(y)=\frac{(-2)^{(n_i+m_i)/2}}{(n_i!m_i!)^{1/2}}\left(\frac{2}{\pi}\right)^{1/2}\frac{(mn)^{1/4}}{(m+n)^{1/2}}$$
$$\times\frac{[(m+n)y-2m]^{n_i/2}[(m+n)y-2n]^{m_i/2}}{(m+n)^{(n_i+m_i)/2}y^{(m_i+n_i+1)/2}}\Gamma\left(\frac{m_i+n_i+1}{2}\right)$$
$$\times F\left(-\frac{m_i}{2},-\frac{n_i}{2};-\frac{(m_i+n_i)}{2}+\frac{1}{2};w\right), \tag{3.22}$$

where

$$w=\frac{(m+n)^2y(y-2)}{[(m+n)y-2m][(m+n)y-2n]}. \tag{3.23}$$

(c) When n_i and m_i are odd

$$S^{n_i,m_i}_{n,m}(y)=-\frac{(-2)^{(n_i+m_i)/2}}{(n_i!\,m_i!)^{1/2}}\frac{2^{3/2}}{\pi^{1/2}}\frac{(nm)^{3/4}}{(n+m)^{3/2}}$$
$$\times\frac{[(m+n)y-2m]^{(n_i-1)/2}[(m+n)y-2n]^{(m_i-1)/2}}{(n+m)^{(n_i+m_i)/2-1}y^{(n_i+m_i+1)/2}}\Gamma\left(\frac{n_i+m_i+1}{2}\right)$$
$$\times F\left(-\frac{(m_i-1)}{2},-\frac{(n_i-1)}{2};-\frac{(m_i+n_i)}{2}+\frac{1}{2};w\right), \tag{3.24}$$

with w given by (3.23).

4. Approaches to the solution of the time dependent Schrödinger equation

The Schrödinger equation for the problem of a hydrogen atom in the presence of a time dependent electric field is given by

$$(H_0+eE(t)z)\Psi(\boldsymbol{r},t)=\mathrm{i}\hbar(\partial/\partial t)\Psi(\boldsymbol{r},t). \tag{4.1}$$

Applying the KS transformation ((2.2) and (2.6)), we obtain:

$$\mathrm{i}\hbar(\partial\Psi/\partial t)(\boldsymbol{u},t)=\left(-\frac{\hbar^2}{2\mu r}\sum_{\alpha=1}^{4}\frac{\partial^2}{\partial u_\alpha^2}-\frac{4e^2}{r}+2eE(t)(u_1u_3+u_2u_4)\right)\Psi(\boldsymbol{u},t) \tag{4.2}$$

with r given by (2.4). If we expand the wavefunctions, in the basis functions given by (2.8) (Chen 1980),

$$\Psi(\boldsymbol{u},t)=\sum_{n,\{n_i\}}a_{n,\{n_i\}}(t)\Psi_{n,\{n_i\}}(\boldsymbol{u}) \tag{4.3}$$

where $\Sigma_{n,\{n_i\}}$ means sum over n and over all possible permutations of n_1, n_2, n_3 and

n_4 subjected to the constraint given by (2.12) and (2.13). The time dependent Schrödinger equation for the $a_{n,\{n_i\}}(t)$'s becomes

$$i\hbar \sum_{n,\{n_i\}} \langle m,\{m_i\}|n,\{n_i\}\rangle \frac{d}{dt} a_{n,\{n_i\}}(t)$$
$$= \sum_{n,\{n_i\}} 4E_n a_{n,\{n_i\}}(t)\langle m,\{m_i\}|n,\{n_i\}\rangle$$
$$+ 2eE(t) \sum_{n,\{n_i\}} a_{n,\{n_i\}}(t)\langle m,\{m_i\}|(u_1u_3+u_2u_4)|n,\{n_i\}\rangle. \tag{4.4}$$

Since $\Psi_{n,\{n_i\}}$ do not form an orthonormal basis, $a_{n,\{n_i\}}(t)$ are not unambiguously defined. In the previous section we showed that, in general

$$\langle m,\{m_i\}|n,\{n_i\}\rangle \neq 0 \qquad \text{for } m \neq n$$

and

$$\langle m,\{m_i\}|n,\{n_i\}\rangle = \delta_{\{m_i\},\{n_i\}} \qquad \text{for } m = n.$$

Therefore the matrix Hamiltonian is not diagonal, even for the unperturbed terms of (4.4). Although, in this way, we lose some generality, we can control our approximations since our matrix elements are exactly calculated. As presented, the problem can be solved using quantum maps if we use for the time dependence a series of δ function pulses. In this case the matrix elements of all powers of z will be necessary, as shown in Hogg and Huberman (1983) and Zavslavsky (1981).

Another approach to the solution of the Schrödinger equation would be to second quantise the Hamiltonian of (4.2) in the basis given by (2.8). It has been shown by Kibler and Négadi (1984), and by Chen (1982), that the unperturbed part of the Hamiltonian reduces to a set of coupled oscillators. In future work we intend to generalise their approach to the perturbed case. The time dependence of the perturbation can be handled by finding a suitable canonical transformation which renders the Hamiltonian time independent (Heitler 1954), or using the Magnus expansion (Pechukas and Light 1965). After this is done the problem may be solved to any desired degree of accuracy.

It is important to notice that we have not discussed the continuum states of the hydrogen atom which are necessary to calculate the ionisation rate. Barut *et al* (1979) and Kibler and Négadi (1983b) showed that these continuum states in three dimensions are also connected with continuum states of a four-dimensional harmonic oscillator with negative potential energy, accompanied by the same constraint. Studies of the matrix elements between continuum and discrete states is in progress.

5. Summary

The problem of the hydrogen atom in the presence of a time dependent electric field poses great computational difficulties. To solve it, we suggest as an alternative method, the use of the four-dimensional harmonic oscillator representation of the hydrogen atom (Boiteux 1973, Kibler and Négadi 1983a, b, 1984, Chen 1980). With this problem in mind, we present the first calculation of the matrix elements of $z^k (k = 1, 2, 3, \ldots)$ between four-dimensional harmonic oscillator states of different frequencies. These can be generated from a single basic matrix element: $\langle m, m_i/n, n_i\rangle$, for which we find explicit expressions (3.13)-(3.16), and (3.19)-(3.24). With these results, the problem

of the hydrogen atom in a time varying external electric field can be solved to any desired degree of accuracy, as outlined in § 4. Finding adequate solutions to this problem is important because of recent experimental evidence concerning the existence of chaos in this type of system (Bayfield *et al* 1977).

Acknowledgments

I am grateful to Drs J Sak and B A Huberman for critical reading of the manuscript, and interesting suggestions. I thank CNPq of Brazil for a Research Fellowship. I also gratefully acknowledge the hospitality and support of the Physics Department at Rutgers University.

References

Barut A O, Schneider C K E and Wilson R 1979 *J. Math. Phys.* **20** 2244
Bayfield J E, Gardner L D and Koch P M 1977 *Phys. Rev. Lett.* **39** 76
Blümel R and Smilansky U 1984 *Phys. Rev. Lett.* **52** 137
Boiteux M 1973 *Physica* **65** 381
—— 1982 *J. Math. Phys.* **23** 1311
Chen A C 1980 *Phys. Rev.* A **22** 333
—— 1982 *Phys. Rev.* A **26** 669
Englefield M J 1972 *Group Theory and the Coulomb Problem* (New York: Wiley)
Gradshteyn I S and Ryzhik I M 1980 *Tables of Integrals, Series and Products* (New York: Academic)
Heitler W 1954 *The Theory of Radiation* 3rd edn (Oxford: OUP) p 147
Hogg T and Huberman B A 1983 *Phys. Rev.* A **28** 22
Jensen R V 1982 *Phys. Rev. Lett.* **49** 1365
—— 1984 *Phys. Rev.* A **30** 386
Kibler M and Négadi T 1983a *J. Phys. A: Math. Gen.* **16** 4265
—— 1983b *Lett. Nuovo Cimento* **37** 225
—— 1984 *Phys. Rev.* A **29** 2891
Landau L V 1958 *Quantum Mechanics* (London: Pergamon)
Leopold J G and Percival I C 1979 *J. Phys. B: At. Mol. Phys.* **12** 709
Littman M G, Zimmerman M L and Kleppner D 1976 *Phys. Rev. Lett.* **37** 486
Pechukas P and Light J C 1965 *J. Chem. Phys.* **44** 3897
Zavslavsky G M 1981 *Phys. Rep.* **80** 157