J. Phys. B: At. Mol. Phys. **18** (1985) 2835-2841. Printed in Great Britain

Effect of continuum–continuum interaction on the ionisation rate of a model atom

R Blümel and R Meir

Department of Nuclear Physics, Weizmann Institute of Science, Rehovot 76100, Israel

Received 2 October 1984

Abstract. A one-dimensional model atom consisting of an attractive δ function at the origin is subjected to a train of δ kicks modelling microwave (laser) ionisation of a real atom. The continuum is taken into account in various approximations which are finally compared with the full (numerical) solution of the model. It is shown that neglecting continuum-continuum interactions is an excellent approximation in the case of kicks of alternating sign.

In this paper we study a simple one-dimensional (1D) model of an atom in an external time periodic field. The motivation for this study is the desire to understand the influence of continuum effects on the ionisation rates of real atoms. Even for the simplest atoms, continuum effects can be taken into account only approximately. However, it is known that a model atom consisting of a δ function at the origin is exactly solvable (numerically) both for static (Geltman 1978, Arrighini and Gavarini 1982) and time-dependent (Geltman 1977, Austin 1979) external fields. This model, therefore, offers the opportunity to study the effect of various approximation schemes towards the complete inclusion of the continuum for periodically perturbed atoms.

The system we will be considering consists of a δ atom subjected to a time periodic field in the form of a sequence of δ-function kicks. In our opinion, this is the simplest possible system, incorporating all the essentials of an atom in an external electromagnetic field. It should be emphasised that our approach will not be perturbative, since we want to include physical situations where the laser field is by no means small.

The Hamiltonian of the system consists of a free part H_0, possessing one bound state and a continuum of positive energy states:

$$H_0 = p^2/2m - V_0\delta(x). \tag{1}$$

To this we add a perturbation of the form:

$$V(x, t) = -e\varepsilon x \sum_{n=-\infty}^{\infty} \delta(t/T - n) = -e\varepsilon x \sum_{m=-\infty}^{\infty} \exp\left(\mathrm{i}m\frac{2\pi}{T}t\right). \tag{2}$$

The properly normalised eigenfunctions of the Hamiltonian H_0 consist of three parts (Brownstein 1975):

(i) the bound-state wavefunction

$$\psi_{\mathrm{B}}(x) = \gamma^{1/2}\exp(-\gamma|x|)$$

where $\gamma = mV_0/\hbar^2$ with energy $E_{\mathrm{B}} = -\hbar^2\gamma^2/2m$;

(ii) negative-parity continuum wavefunctions

$$\psi_k^{(-)}(x) = \pi^{-1/2} \sin(kx) \qquad k > 0$$

and

(iii) positive-parity continuum wavefunctions

$$\psi_k^{(+)}(x) = \pi^{-1/2}[1 + (k/\gamma)^2]^{-1/2}[k\gamma^{-1} \cos(kx) - \sin(k|x|)] \tag{3}$$

with energies $E_k = \hbar^2 k^2/2m$, respectively.

Initially, i.e. shortly before the first kick, our 'atom' is in its ground state. The time evolution for $t > 0$ can be written as a quantum map (Berry *et al* 1979) which gives the wavefunction shortly before kick number $(n+1)$ in terms of the wavefunction shortly before kick number n:

$$|\psi_{n+1}\rangle = \exp\left(-\frac{i}{\hbar} H_0 T\right) \exp\left(\frac{i}{\hbar} e\varepsilon x T\right)|\psi_n\rangle. \tag{4}$$

As we are primarily interested in the depletion (ionisation) of the ground state due to the perturbing field (2), it is useful to divide the total Hilbert space into bound and continuum subspaces with corresponding projection operators $P = |\psi_B\rangle\langle\psi_B|$ and $Q = 1 - P$. If we denote the time evolution operator over one period by U, we may express the quantum map in the following form (Blümel and Smilansky 1984):

$$\begin{aligned} |P\psi_{n+1}\rangle &= U_{PP}|P\psi_n\rangle + U_{PQ}|Q\psi_n\rangle \\ |Q\psi_n\rangle &= U_{QP}|P\psi_{n-1}\rangle + U_{QQ}|Q\psi_{n-1}\rangle = \sum_{j=1}^{n} (U_{QQ})^{j-1} U_{QP}|P\psi_{n-j}\rangle \end{aligned} \tag{5}$$

where U_{PP}, $U_{PQ}\ldots$ stand for PUP, $PUQ\ldots$ respectively.

From the above relations we get the time evolution of the bound state, involving the bound-space wavefunction alone, at the expense of introducing long-time memory terms:

$$|P\psi_{n+1}\rangle = U_{PP}|P\psi_n\rangle + U_{PQ} \sum_{j=1}^{n} (U_{QQ})^{j-1} U_{QP}|P\psi_{n-j}\rangle. \tag{6}$$

Taking the scalar product of (6) with $\langle\psi_B|$ we arrive at an equivalent equation for the time evolution of the bound state amplitudes $a_n = \langle\psi_B|\psi_n\rangle$:

$$a_{n+1} = \langle\psi_B|U|\psi_B\rangle a_n + \sum_{j=1}^{n} \langle\psi_B| U_{PQ}(U_{QQ})^{j-1} U_{QP}|\psi_B\rangle a_{n-j}. \tag{7}$$

Two approximation schemes are possible at this stage. The most primitive one would be to neglect all the memory terms ('never come back' approximation). In this case the bound-state amplitudes evolve according to:

$$a_{n+1} = \langle\psi_B|U|\psi_B\rangle a_n. \tag{8}$$

The matrix element is easily evaluated:

$$\begin{aligned} \langle\psi_B|U|\psi_B\rangle &= \langle\psi_B| \exp[-(i/\hbar)H_0 T] \exp[(i/\hbar)e\varepsilon x T]|\psi_B\rangle = e^{i\tau}\langle\psi_B| \exp(i\beta(\gamma x))|\psi_B\rangle \\ &= \exp(i\tau)[1 + (\beta/2)^2]^{-1} \end{aligned} \tag{9}$$

where

$$\tau = \frac{T}{\hbar}\frac{\hbar^2\gamma^2}{2m} = -\frac{1}{\hbar} E_B T \qquad \text{and} \qquad \beta = \frac{e\varepsilon T}{\hbar\gamma}$$

are dimensionless parameters, proportional to the period and strength of the perturbation.

The mapping (8) of the bound-state amplitudes implies an exponential decay of the bound-state probability

$$P_B(n) = |a_n|^2 = \left(\frac{1}{[1+(\beta/2)^2]^2}\right)^n = \exp(-\lambda n) \tag{10}$$

with decay rate $\lambda = 2\ln[1+(\beta/2)^2]$.

Next we approximate the evolution operator in the continuum by free propagation, i.e.

$$U_{QQ} \simeq \sum_{\pi} \int dk |\psi_k^{(\pi)}\rangle \exp\left(-\frac{i}{\hbar} E_k T\right)\langle\psi_k^{(\pi)}|. \tag{11}$$

This amounts to neglecting all transitions in the continuum, i.e. the continuum components of the wavefunction do not 'feel' the kicks.

In this approximation, (7) can be written as:

$$a_{n+1} = \exp(i\tau)\left(\frac{1}{1+(\beta/2)^2} a_n + \sum_{j=1}^{n} \sum_{\pi} M^{(\pi)}(\beta, j\tau) a_{n-j}\right) \tag{12}$$

where we have introduced the memory integrals $M^{(-)}(\beta, \tau)$ and $M^{(+)}(\beta, \tau)$:

$$M^{(\pi)}(\beta, \tau) = \int_0^\infty dk \langle\psi_B| \exp[i\beta(\gamma x)]|\psi_k^{(\pi)}\rangle\langle\psi_k^{(\pi)}| \exp[i\beta(\gamma x)]|\psi_B\rangle \exp[-i(k/\gamma)^2\tau]. \tag{13}$$

The matrix elements in (13) are given by:

$$\langle\psi_B| \exp[i\beta(\gamma x)]|\psi_k^{(-)}\rangle = \frac{4i\beta}{(\pi\gamma)^{1/2}} \frac{(k/\gamma)}{[1+(k/\gamma-\beta)^2][1+(k/\gamma+\beta)^2]} \tag{14}$$

and

$$\langle\psi_B| \exp[i\beta(\gamma x)]|\psi_k^{(+)}\rangle = \frac{4\beta^2}{(\pi\gamma)^{1/2}} \frac{1}{[1+(k/\gamma)^2]^{1/2}} \frac{(k/\gamma)}{[1+(k/\gamma-\beta)^2][1+(k/\gamma+\beta)^2]}. \tag{15}$$

We note that the amplitudes for transitions from the bound state to the positive-parity continuum states contain an additional factor of β, which for small β, hinder transitions to the positive-parity continuum. This in turn implies a mitigation of the effects of the positive-parity memory terms.

Equation (12) can now be used to map the amplitudes forward in time, obtaining $P_B(n)$. Although inclusion of the memory terms sometimes gave an oscillatory decay of $P_B(n)$, we found that on the average it was still exponential, i.e. $P_B(n) \sim \exp(-\lambda n)$, where λ was obtained by a least-squares fit.

In figure 1 we have plotted the decay rates predicted by (8) and (12) as a function of the frequency $\omega = 2\pi/\tau$. The smooth full curve shows the result including all the memory terms in equation (12). We observe thresholds at fractions of the basic dimensionless frequency $\omega_B = 2\pi/\tau_B = 1$, which correspond to single-photon transitions to the continuum induced by higher harmonics of the perturbation (2). For small frequencies (large τ) both approximations yield essentially identical results, the full curve oscillating with ever smaller amplitude around the never-come-back straight line (broken line in figure 1). This result is intuitively clear. As the time between kicks gets longer the wavepackets ejected into the continuum by the action of a δ kick are

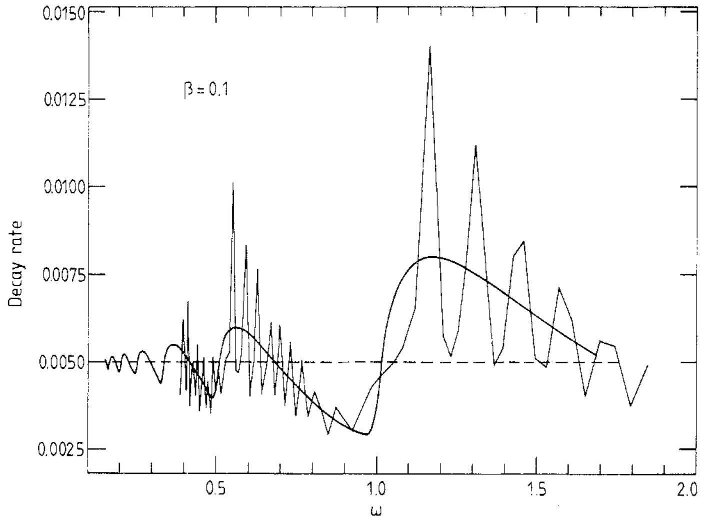

Figure 1. Decay rates calculated in various approaches over 30 cycles of the external field (2).

able to travel further away from the origin. Thus they reduce their overlap with the ground-state wavefunction and avoid being trapped back by another kick. Memory effects should therefore die out in the small-frequency (long-τ) limit.

To get a more quantitative idea of the long-time behaviour of the memory integrals, we calculated them analytically to lowest order in β obtaining:

$$\begin{aligned} M^{(-)}(\beta, j\tau) &\sim \beta^2 \frac{1}{j\tau(j\tau)^{1/2}} + O(\beta^4) \\ M^{(+)}(\beta, j\tau) &\sim \beta^4 \frac{1}{j\tau(j\tau)^{1/2}} + O(\beta^6). \end{aligned} \tag{16}$$

We see that the memory not only dies with τ but also as a function of the memory time j. This decay, however, is very slow and cutting the sum in (12) to only a few memory terms is certainly a bad approximation if (due to a small τ) the memory is at all important.

It should be mentioned that although the approximate U_{QQ} in (11) is a unitary operator in the Q space, the approximation (11) violates over all conservation of probability in the combined $(P+Q)$ space. However, in all the reported calculations, this violation turned out to be exceedingly small, having no effect on the decay rate.

The full solution of the problem, including the complete effects of the continuum, cannot easily be obtained within the framework of the projection operator formalism. The simplest way to incorporate these effects is by putting the system into a box of size $2L$, where L is large enough to guarantee convergence of the results (Austin 1979). As a consequence, the ground-state wavefunction is not at all affected by the finite size of the box, and is still given by:

$$\varphi_B(x) = \gamma^{1/2} \exp(-\gamma|x|). \tag{17}$$

Demanding that the 'continuum' wavefunctions vanish at the boundaries of the box, we obtain the following discrete set of functions:

$$\varphi_n^{(-)}(x)=\gamma^{1/2}\frac{1}{(\gamma L)^{-1/2}}\sin(k_n^{(-)}x) \tag{18}$$

where $k_n^{(-)}=n\pi/L$, $n=1,2,3,\ldots$ and

$$\varphi_n^{(+)}(x)=\gamma^{1/2}\{[1+(k_n^{(+)}/\gamma)^2][\gamma L+\cos^2(k_n^{(+)}L)]-2\}^{-1/2} \times\left(\frac{k_n^{(+)}}{\gamma}\cos(k_n^{(+)}x)-\sin(k_n^{(+)}|x|)\right) \tag{19}$$

where $k_n^{(+)}$ are obtained as roots of the equation:

$$k_n^{(+)}=\gamma\tan(Lk_n^{(+)}). \tag{20}$$

Expanding the full wavefunction after the nth kick in terms of the basis-functions φ_{B}, $\varphi_n^{(-)}$ and $\varphi_n^{(+)}$:

$$\psi_n(x)=a_n\varphi_{\mathrm{B}}(x)+\sum_j b_n^j\varphi_j^{(-)}(x)+\sum_j c_n^j\varphi_j^{(+)}(x) \tag{21}$$

we obtain the mapping:

$$\begin{aligned} a_{n+1}&=\langle\varphi_{\mathrm{B}}|U|\varphi_{\mathrm{B}}\rangle a_n+\sum_j\langle\varphi_{\mathrm{B}}|U|\varphi_j^{(-)}\rangle b_n^{(j)}+\sum_j\langle\varphi_{\mathrm{B}}|U|\varphi_j^{(+)}\rangle c_n^{(j)}\\ b_{n+1}^{(i)}&=\sum_j\langle\varphi_i^{(+)}|U|\varphi_j^{(-)}\rangle b_n^{(j)}+\sum_j\langle\varphi_i^{(+)}|U|\varphi_j^{(+)}\rangle c_n^{(j)}\end{aligned} \tag{22}$$

and a similar equation for the c coefficients.

The 'spiky' curve in figure 1 shows the decay rate for the case where we included the continuum-continuum effects by applying the discrete mapping (22). The smooth curve interpolating it (no continuum-continuum transitions) was reproduced by setting:

$$\langle\varphi_i^{(\pi)}|\exp[\mathrm{i}\beta(\gamma x)]|\varphi_j^{(\sigma)}\rangle\simeq\delta_{\pi\sigma}\delta_{ij}. \tag{23}$$

As we see, the inclusion of continuum-continuum effects leads to a much richer behaviour in the decay rate. In order to understand this we calculated analytically the wavefunction immediately after the first kick, and found it to consist of two wavepackets travelling in opposite directions. If no continuum-continuum interactions are permitted, each kick generates two more packets. The packets travelling to the left do not interfere with those travelling to the right. Including continuum-continuum effects 'pushes' probability from the left to the right, causing frequency-dependent constructive (destructive) interference within the range of the bound-state wavefunction. As the probability to be trapped back depends on the amplitude of the continuum wavefunction in the vicinity of the origin, these interferences must lead to the observed spiky behaviour of the decay rate.

Closer to real microwave (laser) perturbations is a train of δ-function kicks, where the sign of the strength alternates from kick to kick:

$$\begin{aligned} V(x,t)&=-e\varepsilon x\sum_{n=-\infty}^{\infty}\left[\delta\left(\frac{t}{T}-n\right)-\delta\left(\frac{t}{T}-n-\frac{1}{2}\right)\right]\\ &=-2e\varepsilon x\sum_{m=-\infty}^{\infty}\exp\left(\mathrm{i}(2m+1)\frac{2\pi}{T}t\right).\end{aligned} \tag{24}$$

In this case, we expect the neglect of continuum–continuum interactions to be even better. This can be intuitively understood by the following classical analogy: a classical electron, moving with constant speed and subjected to a microwave field, will, on the average, neither gain nor lose momentum. Moreover, we do not expect in this case the spiky behaviour observed in figure 1, because the wavepackets to the left of the origin and those to the right are well separated, and evolve more symmetrically.

The time evolution operator over one period of the external field is now given by:

$$U=\exp\left(-\frac{i}{\hbar}H_0\frac{T}{2}\right)\exp\left(-\frac{i}{\hbar}e\varepsilon xT\right)\exp\left(-\frac{i}{\hbar}H_0\frac{T}{2}\right)\exp\left(\frac{i}{\hbar}e\varepsilon xT\right) \quad (25)$$

and again we can approximately solve the mapping (7) in two ways.

(i) Neglect all the memory terms:

$$a_{n+1}=\langle\psi_B|U|\psi_B\rangle a_n \quad (26)$$

with a corresponding decay rate of

$$\lambda=-\ln(|\langle\psi_B|U|\psi_B\rangle|^2) \quad (27)$$

where the matrix element is evaluated with the help of the memory integrals (13):

$$\langle\psi_B|U|\psi_B\rangle=\left(\frac{\exp(i\tau/2)}{1+(\beta/2)^2}\right)^2+\exp(i\tau/2)\left[M^{(+)}\left(\beta,\frac{\tau}{2}\right)-M^{(-)}\left(\beta,\frac{\tau}{2}\right)\right]. \quad (28)$$

The decay rate (27), which is now frequency dependent, is shown as the broken curve in figure 2. As opposed to (2) the perturbation (24) contains only odd harmonics of the field frequency ω and explains the absence of thresholds at even fractions of the bound-state frequency $\omega_B=1$ in figure 2.

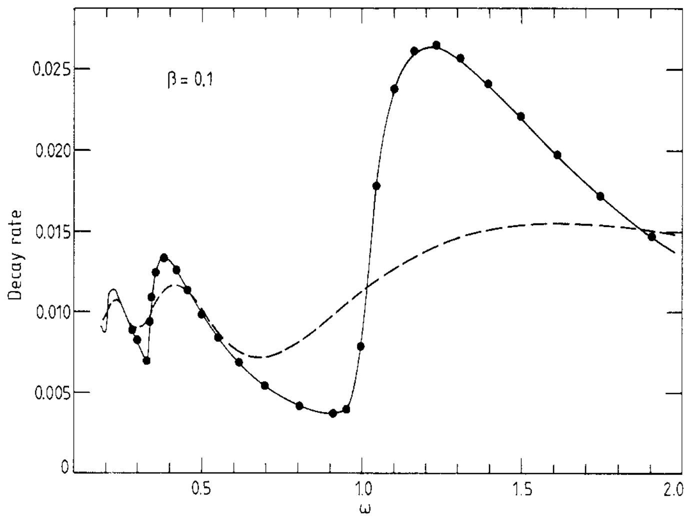

Figure 2. Decay rates in the case of alternate kicks over 15 cycles (30 kicks) of the external field (24).

(ii) Take all memory terms in (7) into account, but approximate U_{QQ} by (11). We obtain:

$$\begin{aligned}\langle\psi_B|U_{PQ}U_{QQ}^{(j-1)}U_{QP}|\psi_B\rangle\\ &\simeq \exp(i\tau/2)[-M^{(-)}(\beta,(j+\tfrac{1}{2})\tau)+M^{(+)}(\beta,(j+\tfrac{1}{2})\tau)]\\ &\quad+2\exp(i\tau)\langle\psi_B|\exp[i\beta(\gamma x)]|\psi_B\rangle[M^{(-)}(\beta,j\tau)+M^{(+)}(\beta,j\tau)]\\ &\quad+\exp(3i\tau/2)\langle\psi_B|\exp[i\beta(\gamma x)]|\psi_B\rangle^2\\ &\quad\times[-M^{(-)}(\beta,(j-\tfrac{1}{2})\tau)+M^{(+)}(\beta,(j-\tfrac{1}{2})\tau)].\end{aligned} \tag{29}$$

The decay rate calculated from (7) with (28) and (29) is shown as the full curve in figure 2 and can be compared with the box results where all the continuum-continuum effects are taken into account (full circles in figure 2). Even though the interaction strength is far from being small (around $\omega=1.2$ we observe 30% ionisation over 30 kicks) the agreement in both rates is astonishingly good. This result of our model investigation should be a strong argument for the neglect of continuum-continuum interactions in microwave (laser) ionisation of real atoms.

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