

phase shift with respect to free waves; from 1 to 4 Ry it is due mostly to the non-Coulomb shape resonance effect in the f -wave channel.¹⁶ Above 4 Ry, the only major variation of β with energy occurs principally because of the Cooper minimum at $\epsilon = 5.6$ Ry and the associated change in sign of R_{l+1} . At still higher energies β is a smooth function of ϵ .

At this point it is worthwhile to point out that this calculation does not treat exchange exactly and omits correlation and spin-orbit effects which may be important.¹⁷ Indications are that exchange effects will not significantly affect the angular distribution.¹⁵ As for the other effects, while they may change the positions of the minima and maxima in β somewhat, it seems unlikely that they could greatly affect the overall oscillatory behavior.

In conclusion, we hope that experimental studies, as well as further theoretical work, will provide more information on this phenomenon.

¹K. Siegbahn *et al.*, *Nova Acta Regiae Soc. Sci. Upsal.* **20**, 1 (1967).

²J. Berkowitz and H. Ehrhardt, *Phys. Lett.* **21**, 531

(1966).

³J. Berkowitz, H. Ehrhardt, and T. Tekaas, *Z. Phys.* **200**, 69 (1967).

⁴M. O. Krause, *Phys. Rev.* **177**, 151 (1969), and private communication.

⁵T. Carlson, private communication.

⁶J. W. McGowan, D. A. Vroom, and A. R. Comeaux, *J. Chem. Phys.* **51**, 5626 (1969).

⁷H. Harrison, *J. Chem. Phys.* **52**, 901 (1970).

⁸J. A. R. Samson, *Bull. Amer. Phys. Soc.* **14**, 950 (1969).

⁹J. A. R. Samson, to be published.

¹⁰R. Schoen, private communication.

¹¹R. Morgenstern, A. Nienaus, and M. Ruf, *Chem. Phys. Lett.* **4**, 635 (1970).

¹²J. Cooper and R. N. Zare, *J. Chem. Phys.* **48**, 942 (1968).

¹³J. Cooper and R. N. Zare, in *Lectures in Theoretical Physics*, edited by S. Geltman, K. Mahanthappa, and W. E. Brittin (Gordon and Breach, New York, 1969), Vol. XI C, p. 317.

¹⁴For details of this calculation see J. W. Cooper, *Phys. Rev.* **128**, 681 (1962); S. T. Manson and J. W. Cooper, *Phys. Rev.* **165**, 126 (1968).

¹⁵S. T. Manson and D. J. Kennedy, *Chem. Phys. Lett.*, **7**, 387 (1970).

¹⁶S. T. Manson, *Phys. Rev.* **182**, 97 (1969).

¹⁷U. Fano, *Comments At. Mol. Phys.* **2**, 30 (1970).

Time Evolution of Simple Quantum-Mechanical Systems.

II. Two-State System in Intense Fields*

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The Schrödinger equation for a two-state quantum-mechanical system with sinusoidal perturbation is numerically integrated with respect to time. From these results a general formula for the induced transition probability (as a function of time, perturbation frequency, and perturbation strength) is extracted.

There has been a recent surge of interest in the properties of quantum systems in intense, coherent radiation fields.¹⁻³ We present here those preliminary results of a more general investigation which are relevant to this problem.

Consider a two-state system with states $|0\rangle$ and $|1\rangle$; we introduce an external time-dependent driving field in the Hamiltonian:

$$H = H_0 + V \sin(\omega t + \delta),$$

where

$$H_0|0\rangle = 0, \quad H_0|1\rangle = \hbar\omega_0|1\rangle,$$

$$\langle 0|V|0\rangle = \langle 1|V|1\rangle = 0,$$

and

$$\langle 0|V|1\rangle = V_{01} = \langle 1|V|0\rangle.$$

The time-evolution operator in the interaction representation satisfies the Schrödinger equation⁴:

$$i\hbar(\partial/\partial t)U_I(t) = V_I(t)U_I(t). \quad (1)$$

Since all the matrices in (1) are two-by-two, it is a trivial matter to integrate the equation numerically with initial condition $U_I(0) = 1$. In Fig. 1 we show the induced transition probability, $|\langle 1|U_I(t)|0\rangle|^2$, as a function of time for several values of ω/ω_0 , with $\delta = 0$ and the perturbation

strength $|V_{01}|/\hbar\omega_0=0.1$. (This perturbation strength is enormous compared with those in the physical systems to which the two-level system is meant to be an approximation; however, this strength was used in initial runs to induce transitions on a reasonable time scale. It was our expectation, since borne out, that the results for weaker perturbations might be simpler but would not be more complicated.)

It is seen from Fig. 1 that the transition probabilities all have the overall form $a \sin^2(t\pi/\tau)$ modulated by some weaker and higher frequency oscillation. Changing the perturbation phase factor δ (graphs not shown) shifts the phase of the high-frequency component, and slightly shifts the maximum amplitude, but does not alter the overall behavior. For weaker perturbations, the general form is the same with different periods and amplitudes. We may summarize a large number of computations by writing the slowly varying part of the transition probability as

$$|b_{10}(t)|^2 = |\langle 1|U_I(t)|0\rangle|^2 = \frac{(V_{01}/\hbar)^2}{(\omega-\omega_0)^2 + (V_{01}/\hbar)^2} \sin^2\left\{\frac{t}{2}\left[(\omega-\omega_0)^2 + \left(\frac{V_{01}}{\hbar}\right)^2\right]^{1/2}\right\}. \quad (2)$$

Equation (2) is plotted in Fig. 1 as solid lines. The solid line does not go through the "center" of the modulation in every case, but the effect of δ is to shift the modulation such that (2) is effectively an average over phase δ . Nevertheless, (2) fits the overall behavior very well.

One significance of the result (2) is as follows: The maximum amplitude is given by (writing V

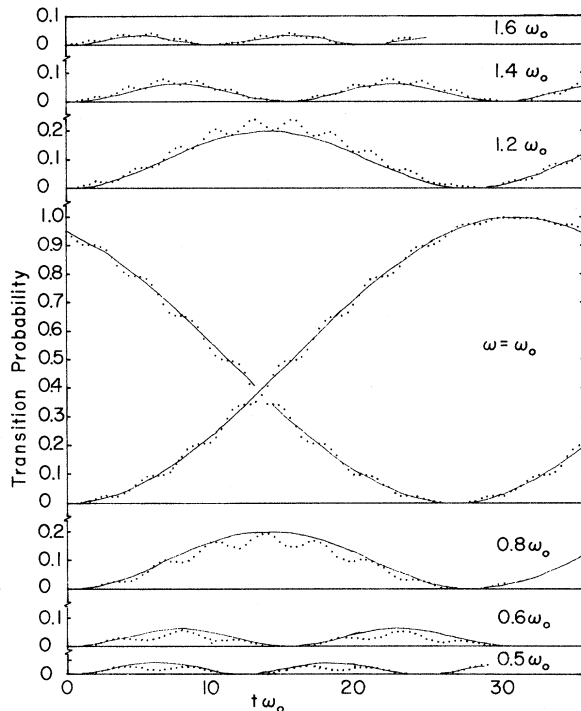


FIG. 1. Graphs of the induced transition probability $|b_{10}(t)|^2 = |\langle 1|U_I(t)|0\rangle|^2$ for a two-level system for various perturbation frequencies ω/ω_0 , with perturbation strength $V_{01}/\hbar=0.1\omega_0$, and perturbation phase $\delta=0$. Dotted lines are numerical integration and solid line is from Eq. (2). (The graph for $\omega=\omega_0$ has been cut at $t\omega_0=36$ and shifted to the origin.)

for V_{01})

$$a = \frac{(V/\hbar)^2}{(\omega-\omega_0)^2 + (V/\hbar)^2}$$

and this occurs at $t=\tau/2$ where

$$\tau = \frac{2\pi\hbar}{V} \left[\frac{(V/\hbar)^2}{(\omega-\omega_0)^2 + (V/\hbar)^2} \right]^{1/2}$$

Thus, if after time $\tau/2$ the transition probability is a , on a long-time basis we are inducing transitions at the rate of

$$R = \frac{2a}{\tau} = \frac{(V/\hbar)^2}{\pi[(\omega-\omega_0)^2 + (V/\hbar)^2]^{1/2}} \quad (3)$$

per unit time. Thus exactly on resonance the "transition rate" is proportional to $|V_{01}|$ rather than $|V_{01}|^2$. Clearly, with ordinary perturbation strengths and light sources, this effect would never be seen; however, with intense, highly monochromatic fields, behavior represented by (3) dominates.

Finally, we note that exactly on resonance the dotted curve in Fig. 1 is, within the plotting accuracy, identical to the approximate result

$$|b^1(t)|^2 = |\langle 1|\exp[(1/i\hbar)\int_0^t V_I(t')dt']|0\rangle|^2.$$

A more detailed discussion will be presented elsewhere.

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¹T. Oka and T. Shimizu, Phys. Rev. A **2**, 587 (1970).

²H. R. Reiss, Phys. Rev. Lett. **25**, 1149 (1970).

³A. Ashkin, Phys. Rev. Lett. **25**, 1321 (1970).

⁴A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), Vol. I, p. 322.