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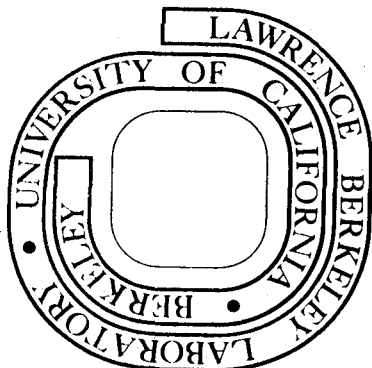
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Interference Effects in Rotational State Distributions;
Propensity and Inverse Propensity*

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Abstract

Semiclassical scattering theory has been used to investigate interference effects in rotational state distributions for inelastic atom-diatom collisions. The $\Delta j = \text{even}$ selection rule for homonuclear molecules is seen semiclassically to be an interference effect, and when this symmetry is weakly broken--i.e., an "almost homonuclear" molecule, one for which the odd anisotropy is much smaller than the even anisotropy--the interference persists in the form of a propensity rule, $\sigma(\text{odd } \Delta j) \ll \sigma(\text{even } \Delta j)$. If the odd anisotropy is sufficiently large, however, one can see an inversion of the normal propensity, i.e., it can happen that $\sigma(\text{odd } \Delta j) > \sigma(\text{even } \Delta j)$. It is suggested that rotationally state selected experiments which resolve this interference structure would be an extremely sensitive measure of the anisotropy in the interaction potential.

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I. Introduction

The primary effect of quantum mechanics in atomic and molecular collision processes is to provide an interference structure about the results given by classical mechanics. There are many examples of this, perhaps the best known one being the interference (and rainbow) structure seen in elastic atom-atom scattering.^{1,2}

Classical S-matrix theory³ is a semiclassical approach that adds the quantum principle of superposition (i.e., interference) to classical mechanics in a general and correct manner and is thus able to describe quantum interference effects in complex--i.e., inelastic and reactive--collision processes. The first application⁴ of classical S-matrix theory, in fact, showed that there is an interference structure in internal state distributions--e.g., the distribution of final vibrational or rotational states after an inelastic or reactive collision--quite analogous to the interference features in the angular distribution for elastic scattering.^{1,2} The physical origin of this interference in internal state distributions is precisely the same as that of interference in elastic scattering: in both cases there is more than one classical trajectory which leads to the specific final state (a specific final internal state or a specific scattering angle), and the net amplitude for the transition is the sum of amplitudes related to each such trajectory; interference between these several classical trajectories results when the net amplitude is squared to obtain cross sections.

The interference features in inelastic and reactive scattering are often quenched,⁵ however, because experimental measurements are rarely

state-selected, and anything less than measurements of completely specified initial and final states involves some averaging that tends to wash out the interference structure. (For elastic atom-atom scattering there are no internal states, so that the differential cross section is the complete measurement in this case.)

In this paper we discuss an interference effect in rotationally inelastic scattering that is often not quenched by averaging. To see its origin, consider rotational excitation of a homonuclear diatomic molecule, e.g., N_2 , by collision with an atom. As is well known, quantum mechanics only allows an even change in the rotational quantum number j . This selection rule, $\Delta j = \text{even}$, is also obtained rigorously in classical S-matrix theory^{3c,6} where it appears as an interference effect; i.e., classical trajectories with odd Δj exist but destructive interference causes the net amplitude for them to be zero. Section II reviews this in more detail.

The interesting situation arises for an "almost homonuclear" diatomic molecule, i.e., a heteronuclear diatomic for which the odd anisotropy is much smaller than the even anisotropy. In this case odd Δj transitions are diminished by destructive interference but yet have finite cross sections. This propensity, or weak selection rule is often not quenched by averages over impact parameter or the initial and final m -components of the rotational state, and has been observed and noted in some calculations.⁷ It is clear that it cannot be properly described by a completely classical theory which does not include interference.^{7,8}

This paper reports calculations we have carried out, using classical S-matrix theory, to illustrate and characterize this propensity rule by systematically varying the relative amounts of the even and odd anisotropies

of representative interaction potentials. Section III describes the results of these calculations.

One particularly interesting, and unexpected effect seen in the calculations is the discovery of an "inverse propensity" effect. As noted, if the odd anisotropy is zero (i.e., a homonuclear molecule), odd Δj transitions have zero cross section, and not surprisingly, increasing the odd anisotropy increases the cross section for odd Δj transitions. This can continue until the cross sections for odd Δj are actually larger than those for even Δj transitions. For a given value of the anisotropy one can sometimes see both the usual propensity (enhanced even Δj transitions) for small Δj and the inverse propensity (enhanced odd Δj transitions) for large Δj . It is clear that experiments that are sufficiently state-selected to observe these effects would be extremely useful in obtaining quantitative information about the anisotropy of the interaction potential.

II. Qualitative Discussion

To see the semiclassical origin of the selection and propensity rules it is sufficient to consider rotational excitation of a plane rotor.^{3c}

The classical Hamiltonian for such a system is

$$H(P,R,j,q) = \frac{P^2}{2\mu} + Bj^2 + V(R,q) \quad , \quad (2.1)$$

where (P,R) are the momentum and coordinates for the translational degree of freedom (with reduced mass μ), and (j,q) are the action-angle variables for the rotational degree of freedom; B is the rotation constant for the rotor. The action variable j is the classical counterpart to the rotational quantum number.

The semiclassical expression for the probability of the $j_1 \rightarrow j_2$ rotational transition is³

$$P_{j_2 \leftarrow j_1} = |S_{j_2, j_1}|^2 \quad , \quad (2.2)$$

where the classical S-matrix element (i.e., the transition amplitude) is given by

$$S_{j_2, j_1} = \sum [2\pi i \frac{\partial j_2(\bar{q}_1, j_1)}{\partial \bar{q}_1}]^{-1/2} \exp[i\phi(j_2, j_1)] \quad , \quad (2.3)$$

(units being used such that $\hbar = 1$), where ϕ is the action integral

$$\phi(j_2, j_1) = - \int_{-\infty}^{\infty} dt [R(t) \frac{d}{dt} P(t) + q(t) \frac{d}{dt} j(t)] \quad , \quad (2.4)$$

and $j_2(\bar{q}_1, j_1)$ is the final value of the rotational angular momentum that results from a classical trajectory with the following initial conditions:

$$j(t_1) = j_1 \quad (\text{an integer}) \quad (2.5a)$$

$$R(t_1) = R_{\max} \quad (\text{an arbitrarily large value}) \quad (2.5b)$$

$$P(t_1) = -\sqrt{2\mu[E - Bj_1^2]} \quad (2.5c)$$

$$q(t_1) = \bar{q}_1 + 2Bj_1 \mu R(t_1)/P(t_1) \quad ; \quad (2.5d)$$

E is the total energy of the system. \bar{q}_1 is evaluated at the root of the equation

$$j_2(\bar{q}_1, j_1) = j_2 \quad (\text{an integer}) \quad , \quad (2.6)$$

and the sum in Eq. (2.3) is a sum of such terms over all values of \bar{q}_1 in the interval $(0, 2\pi)$ that satisfy Eq. (2.6). The reader may consult earlier work³ for more details of this semiclassical theory.

One knows that $j_2(\bar{q}_1)$ (dropping the argument j_1 for notational simplicity) is a periodic function in the interval $(0, 2\pi)$ because \bar{q}_1 and $\bar{q}_1 + 2\pi$ is the same physical initial condition. (In the present example, the angle variable q is the orientation angle of the rotor.) If the rotor is homonuclear (i.e., $V(R, q) = V(R, q+\pi)$), however, then \bar{q}_1 and $\bar{q}_1 + \pi$ are also the same physical initial condition since a rotation by π interchanges the two identical ends of the rotor. The function $j_2(\bar{q}_1)$ is thus periodic in the interval $(0, \pi)$, as shown in Figure 1. In the simplest generic case, therefore, Eq. (2.6) will have 4 roots,

as indicated graphically in Figure 1, so that the S-matrix element will have 4 terms,

$$S_{j_2, j_1} = S_{j_2, j_1}^{(1)} + S_{j_2, j_1}^{(2)} + S_{j_2, j_1}^{(3)} + S_{j_2, j_1}^{(4)}, \quad (2.7)$$

each term being of the form in Equation (2.3). The first and third terms, however, are not independent; the only difference between the two trajectories from which these terms are constructed is that $\bar{q}_1^{(3)} = \bar{q}_1^{(1)} + \pi$, and for all values of time t one thus has

$$R^{(3)}(t) = R^{(1)}(t) \quad (2.8a)$$

$$P^{(3)}(t) = P^{(1)}(t) \quad (2.8b)$$

$$j^{(3)}(t) = j^{(1)}(t) \quad (2.8c)$$

$$q^{(3)}(t) = q^{(1)}(t) + \pi \quad (2.8d)$$

It then follows that

$$\left. \frac{\partial j^{(3)}(\bar{q}_1)}{\partial \bar{q}_1} \right|_{\bar{q}_1 = \bar{q}_1^{(3)}} = \left. \frac{\partial j^{(1)}(\bar{q}_1)}{\partial \bar{q}_1} \right|_{\bar{q}_1 = \bar{q}_1^{(1)}}, \quad (2.9)$$

and

$$\begin{aligned} \phi_{j_2, j_1}^{(3)} &\equiv - \int_{-\infty}^{\infty} dt [R^{(3)}(t) \frac{d}{dt} P^{(3)}(t) + q^{(3)}(t) \frac{d}{dt} j^{(3)}(t)] \\ &= - \int_{-\infty}^{\infty} dt [R^{(1)}(t) \frac{d}{dt} P^{(1)}(t) + (q^{(1)}(t) + \pi) \frac{d}{dt} j^{(1)}(t)] \\ &= \phi_{j_2, j_1}^{(1)} - \pi \int_{-\infty}^{\infty} dt \frac{d}{dt} j^{(1)}(t), \end{aligned}$$

or

$$\phi_{j_2, j_1}^{(3)} = \phi_{j_2, j_1}^{(1)} - \pi(j_2 - j_1) \quad , \quad (2.10)$$

so that

$$S_{j_2, j_1}^{(3)} = S_{j_2, j_1}^{(1)} e^{-i\pi\Delta j} \quad , \quad (2.11)$$

where

$$\Delta j = j_2 - j_1 \quad .$$

The second and fourth terms in Eq. (2.7) are related in a similar way,

$$S_{j_2, j_1}^{(4)} = S_{j_2, j_1}^{(2)} e^{-i\pi\Delta j} \quad , \quad (2.12)$$

so that the net S-matrix element is

$$S_{j_2, j_1} = (1 + e^{-i\pi\Delta j}) (S_{j_2, j_1}^{(1)} + S_{j_2, j_1}^{(2)}) \quad . \quad (2.13)$$

The rigorous selection rule is thus apparent for the homonuclear case:

$$S_{j_2, j_1} = 0 \quad , \quad \Delta j \text{ odd} \quad (2.14a)$$

$$= 2(S_{j_2, j_1}^{(1)} + S_{j_2, j_1}^{(2)}) \quad , \quad \Delta j \text{ even} \quad , \quad (2.14b)$$

which we again emphasize is a direct consequence of interference.

Consider now what happens if a small odd anisotropy is introduced in the potential $V(R,q)$ (e.g., a small term proportional to $\cos q$): the shape of the function $j_2(\bar{q}_1)$ will be slightly perturbed and cease to be identical in the intervals $(0,\pi)$ and $(\pi,2\pi)$, as seen in Figure 1. The first and third terms in Eq. (2.7) will thus not cancel identically for odd Δj as before, although there will still be considerable destructive interference if the symmetry of $j_2(\bar{q}_1)$ is only slightly perturbed. The transition probability for odd Δj transitions, though still small, will now be finite.

The degree to which the symmetry of $j_2(\bar{q}_1)$ about π is broken is directly related to the amount of odd anisotropy in the interaction potential. In the next section we present some sample calculations which show the propensity effects as a function of relative magnitudes of the even and odd anisotropies in the potential.

III. Example Calculations

a. The Helicity Conserving Approximation.

To keep the calculations as simple as possible we decided to carry them out within the framework of the "j_z conserving" approximation^{9,10} that has been used recently in quantum mechanical coupled channel calculations and found to be reasonably accurate in a number of cases (particularly so for integral cross sections that are averaged over initial and final m-components of the rotational states). Although there may be cases for which this approximation is inadequate, it should suffice to demonstrate the interference effects in rotational excitation that were discussed in the previous section.

The complete (classical) Hamiltonian in the helicity representation for an atom-rigid rotor system has been given before¹¹ and is

$$H(P,R,j,q,K,q_K) = \frac{P^2}{2\mu} + Bj^2 + V(R,\gamma) \\ + (2\mu R^2)^{-1} [J^2 - K^2 + j^2 - K^2 + 2\sqrt{J^2 - K^2}\sqrt{j^2 - K^2}\cos q_K] \quad , \quad (3.1)$$

where (R,P) are the coordinate and momentum for relative translational motion, (j,q) are the action-angle variables for the rotational degree of freedom, and (K,q_K) are the action angles for the helicity; i.e., K is the component of total angular momentum along the relative coordinate vector, $K = \vec{J} \cdot \hat{R}$ and q_K is the angle variable conjugate to it. J is the total angular momentum, which is conserved, and B is the rotation constant for the rotor. γ is the angle between the center of mass coordinate vector and the vector along the rotor,

$$\cos\gamma = \hat{r} \cdot \hat{R} \quad ,$$

and is given in terms of the canonical variables by¹¹

$$\cos\gamma = \sqrt{1 - K^2/j^2} \cos\alpha \quad . \quad (3.2)$$

The helicity-or j_z -conserving approximation^{9,10} is to assume that K is conserved, for which it is necessary to replace the Hamiltonian in Eq. (3.1) by one that does not involve the angle α_K . The most obvious way to do this is simply to average H in Eq. (3.1) over α_K (this corresponds to taking the diagonal matrix elements of the Hamiltonian operator in quantum mechanics¹⁰), whereby the quantity in square brackets in Eq. (3.1) is replaced by

$$[J^2 + j^2 - 2K^2] \quad .$$

(Augustin and Rabitz¹² have also noted that this is the classical version of the " j_z conserving" approximation.) More recently, however, arguments^{13,14} have been presented, with numerical examples to support them, that the term in square brackets, the orbital angular momentum ℓ^2 , should be taken as a constant and all reference to the total angular momentum J discarded. We have done this. Thus the classical Hamiltonian we have used is

$$H(P, R, j, \alpha) = \frac{P^2}{2\mu} + \frac{\ell^2}{2\mu R^2} + B j^2 + V(R, \gamma) \quad . \quad (3.3a)$$

Furthermore, since we have only considered transitions with $j_1 = 0$, only the case $K = 0$ need be treated, so that Eq. (3.2) becomes

$$\cos \gamma = \cos q$$

i.e.,

$$\gamma = q \quad (3.3b).$$

This approximate Hamiltonian, Eq. (3.3), one recognizes as the same as that for the plane rotor discussed in Section II with the addition of the centrifugal term $\ell^2/2\mu R^2$.

The classical S-matrix elements obtained from the Hamiltonian in Eq. (3.3) depend parametrically on ℓ , $S_{j_2, j_1}(\ell)$, and in terms of them the cross section for the $j_1 \rightarrow j_2$ transition is

$$\sigma_{j_2 \leftarrow j_1} = \frac{\pi}{k_1^2 (2j_1 + 1)} \sum_{\ell=0}^{\infty} (2\ell + 1) |S_{j_2, j_1}(\ell)|^2 \quad ; \quad (3.4)$$

in practice this sum is taken as an integral which is evaluated by quadrature.

b. The Initial Value Representation.

From the qualitative discussion in Section II it is clear that typical S-matrix elements in the present example will have four terms contributing to them. For quantitative purposes it would be necessary to use a uniform asymptotic approximation³ for them, rather than the primitive semiclassical approximation discussed in Section II. Although uniform asymptotic expressions for this situation have been discussed,¹⁵ it seemed simpler to us to employ the initial value representation.⁴ This

integral representation for the classical S-matrix has the advantage that if it is evaluated directly (i.e., numerically) it automatically "uniformizes" the result in an approximate fashion. It has been seen in a number of examples^{4,16} to be quite accurate for processes that are not strongly classically forbidden, i.e., that have transition probabilities not too small, $\geq 10^{-2}$.

The initial value representation for the classical S-matrix is⁴

$$S_{j_2, j_1} = (2\pi)^{-1} \int_0^{2\pi} d\bar{q}_1 \left[\frac{\partial \bar{q}_2(\bar{q}_1, j_1)}{\partial \bar{q}_1} \right]^{1/2} \exp\{i\phi(\bar{q}_1, j_1) + i \bar{q}_2(\bar{q}_1, j_1) [j_2(\bar{q}_1, j_1) - j_2]\} \quad (3.5)$$

where ϕ and $j_2(\bar{q}_1, j_1)$ are the same quantities as in Section II, and \bar{q}_1 is the initial phase in Eq. (2.5d); similarly the final phase \bar{q}_2 is defined as

$$\bar{q}_2 = \lim_{t \rightarrow \infty} [q(t) - 2Bj(t) \mu R(t)/P(t)] .$$

The integral over \bar{q}_1 was evaluated by fitting the functions (suppressing the argument j_1) $j_2(\bar{q}_1)$, $\bar{q}_2(\bar{q}_1)$, and $\phi(\bar{q}_1) + \bar{q}_1 [j_2(\bar{q}_1) - j_1]$ --which are all periodic in the interval $(0, 2\pi)$ --to Fourier series. Typically ~ 32 classical trajectories were run at equally spaced increments of \bar{q}_1 to generate a thirty-two term Fourier expansion for them. Using these Fourier series for the functions involved, the integrand of Eq. (3.5) could then be accurately evaluated at any value of \bar{q}_1 , allowing one to use a high order quadrature to evaluate the integral without requiring a large number of classical trajectories to be run.

c. Interaction Potential and Results.

An anisotropic Lennard-Jones potential,

$$V(R, \gamma) = V_0(R) [1 + a_1 P_1(\cos \gamma) + a_2 P_2(\cos \gamma)]$$

where

$$V_0(R) = \epsilon [(R_m/R)^{12} - 2(R_m/R)^6] \quad , \quad (3.6)$$

qualitatively represents many atom-diatom systems and is a useful form without a large number of arbitrary parameters. It is convenient to measure energy in units of ϵ and distance in units of R_m . For the translational energy E and the rotation constant B we have used

$$E/\epsilon = 150 \quad (3.7a)$$

$$B/\epsilon = 0.1 \quad . \quad (3.7b)$$

The anisotropy parameters a_1 and a_2 are the variables of interest to explore the interference effects discussed in Section II.

The first set of calculations are with anisotropy parameters

$$a_1 = 0.15$$

$$a_2 = 1.2 \quad ,$$

and illustrate the rigorous selection rule for the homonuclear case ($a_1 = 0$) and the weak selection, or propensity rule, for the almost homonuclear ($a_1 = 0.15$) case. Figure 1 shows the rotational quantum

number function $j_2(\bar{q}_1)$; as discussed in Section II it is identical in the intervals $(0, \pi)$ and $(\pi, 2\pi)$ for the homonuclear case and slightly distorted when this symmetry is broken. The cross sections for these two cases are shown in Figure 2 and are a clear illustration of the interference effect being discussed. In this calculation rotational excitation to $j_2 = 16$ is classically allowed for low orbital angular momentum ℓ , and one sees in Figure 2 that the propensity rule persists even into the classically forbidden region $j_2 > 16$.

Interference effects of this type have been seen in the calculations of Thaddeus and Green¹⁷ for the case of He + CO collisions. The interference nature of these effects was pointed out by Augustin and Miller,⁷ who also showed that although a purely classical calculation (the usual quasi-classical Monte Carlo method) cannot reproduce the interference structure, it can reproduce the average rotational excitation spectrum well. The inability of purely classical calculations to describe these interference effects has also been discussed by Brumer.⁸

Before carrying out these calculations we had expected that the interference structure would be quenched as the odd anisotropy parameter a_1 is increased relative to the even anisotropy parameter a_2 . Although this does happen eventually, interesting things are observed before the interference is quenched completely.

Figure 3 shows the cross sections for the values $a_1 = 0.3$ and 0.4 , still with $a_1 = 1.2$. One notes two distinct regions of behavior: for small j_2 the ordinary propensity rule is observed, but at large j_2 the situation is reversed, odd Δj transitions are enhanced. The cross sections for the still larger values of the odd anisotropy $a_1 = 0.7$ and 0.8 , shown

in Figure 4, show the inverse propensity even at small j_2 , and after a transition region show the usual propensity at the largest values of j_2 . Calculations with other combinations of a_1 and a_2 show the same qualitative behavior if a_2 is increased while holding a_1 constant.

This rather surprising behavior can be understood in terms of the same arguments about interfering trajectories that were used to describe the ordinary propensity effects in the almost homonuclear case ($a_1 \ll a_2$) in Section II. Since in the present example the interference between trajectories 1 and 2 and between 3 and 4 causes no observable interference structure--either it is quenched by the sum over ℓ or does not vary significantly with j_2 --it is useful to group terms 1 and 2 and terms 3 and 4 of Eq. (2.7) together,

$$S_{j_2, j_1} = S_{j_2, j_1}^{(I)} + S_{j_2, j_1}^{(II)}, \quad (3.8)$$

where

$$S_{j_2, j_1}^{(I)} = S_{j_2, j_1}^{(1)} + S_{j_2, j_1}^{(2)}$$

$$S_{j_2, j_1}^{(II)} = S_{j_2, j_1}^{(3)} + S_{j_2, j_1}^{(4)}$$

The two terms in Eq. (3.8) are complex numbers and may thus be written as

$$S_{j_2, j_1}^{(I)} = p_I^{1/2} e^{i\phi_I}$$

$$S_{j_2, j_1}^{(II)} = p_{II}^{1/2} e^{i\phi_{II}},$$

where p_I and p_{II} are non-oscillatory; thus

$$\begin{aligned} |S_{j_2, j_1}|^2 &= |p_I^{1/2} e^{i\phi_I} + p_{II}^{1/2} e^{i\phi_{II}}|^2 \\ &= p_I + p_{II} + 2(p_I p_{II})^{1/2} \cos(\Delta\phi) \end{aligned} \quad (3.9)$$

where

$$\Delta\phi = \phi_{II} - \phi_I .$$

As discussed before, if $a_1 = 0$ (the homonuclear limit) one has

$$p_I = p_{II} \equiv p \quad (3.10a)$$

$$\Delta\phi = -\pi\Delta j \quad , \quad (3.10b)$$

so that Eq. (3.9) becomes

$$|S_{j_2, j_1}|^2 = 2p[1 + \cos(\pi\Delta j)] \quad ,$$

from which the rigorous selection rule follows. As a_1 increases, p_I and p_{II} are no longer equal, and also the phase difference $\Delta\phi$ varies from that in Eq. (3.10b). In fact our computational results indicate that for $a_2 = 1.2$ the phase difference varies with Δj and a_1 approximately as

$$\Delta\phi \approx -\pi\Delta j (1 + .2 a_1) \quad . \quad (3.11)$$

For $a_1 = 0.4$ and $j_2 = 12$, therefore,

$$\Delta\phi \approx -\pi\Delta j + \pi \quad ,$$

i.e., the interference is exactly out of phase with that predicted by the ordinary propensity (which stems from $\Delta\phi = -\pi\Delta j$). The dependence of $\Delta\phi$ on a_1 and Δj in Eq. (3.11) qualitatively explains all the interference behavior observed in our calculations.

Eventually, however, the interference structure is quenched for $a_2 \ll a_1$. This is shown in Figure 5 for the case $a_1 = 1.0$ and $a_2 = 0.5$.

IV. Concluding Remarks

Semiclassical theory provides a natural and useful way to understand quantum interference effects in internal state distributions. These are completely analogous to the interference effects in angular distributions for elastic (or inelastic) scattering which are also usefully described semiclassically.

The model calculations described in Section III show that interesting interference structure in rotational state distributions need not be quenched by sums over orbital angular momentum and averages over the initial and final m components of the rotational states. Semiclassical theory provides a convenient means of calculating these cross sections (although this could also have been done quantum mechanically). As in elastic scattering, however, the most important contributions of semiclassical theory is the insight into the physical origin of the quantum effects that it provides.

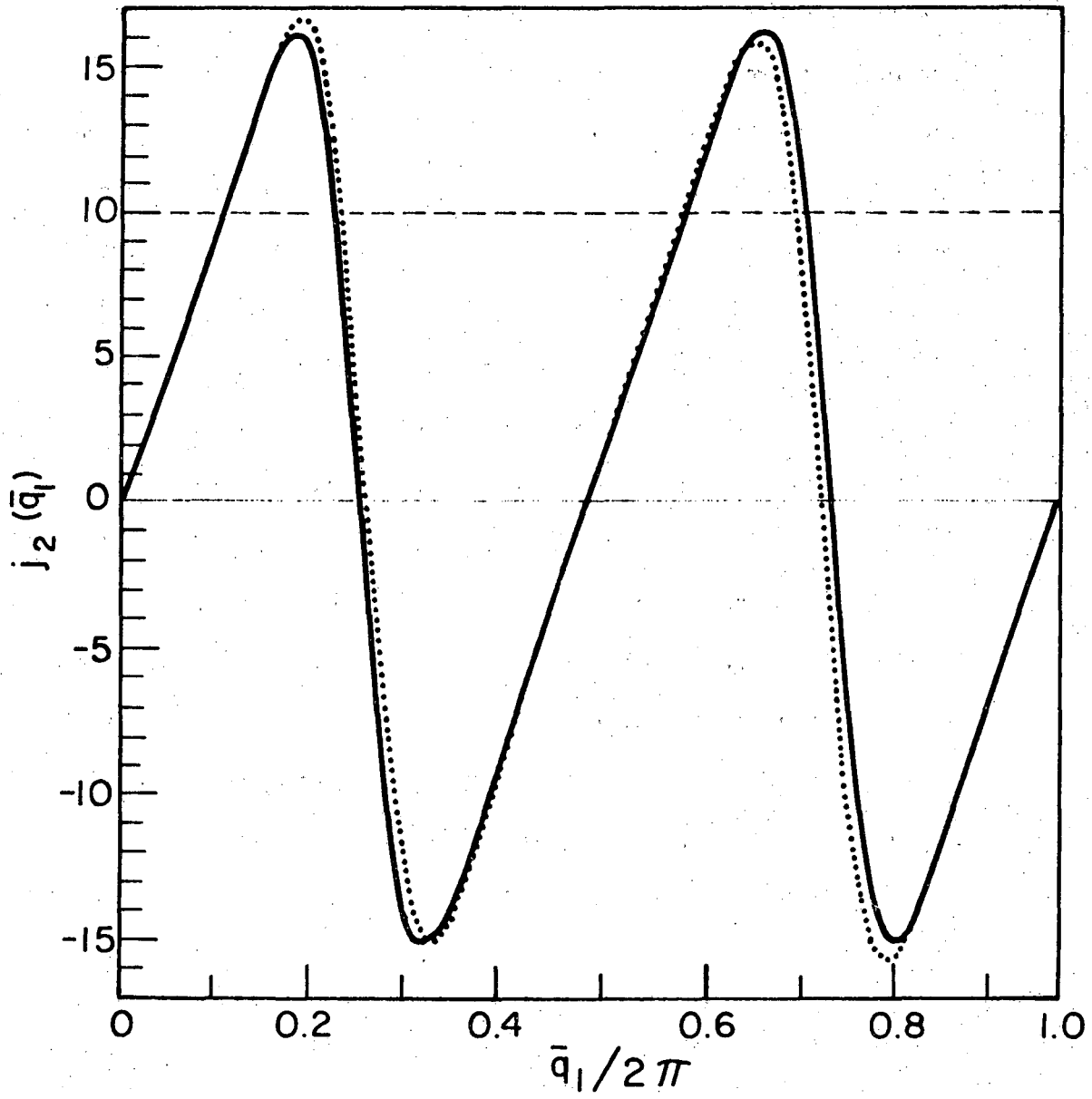
The most unexpected effect seen in this example is that the interference structure need not be quenched as soon as the weak selection rule (small cross sections for odd Δj transitions) is violated. Experimental observations of these interference effects would be quite exciting.

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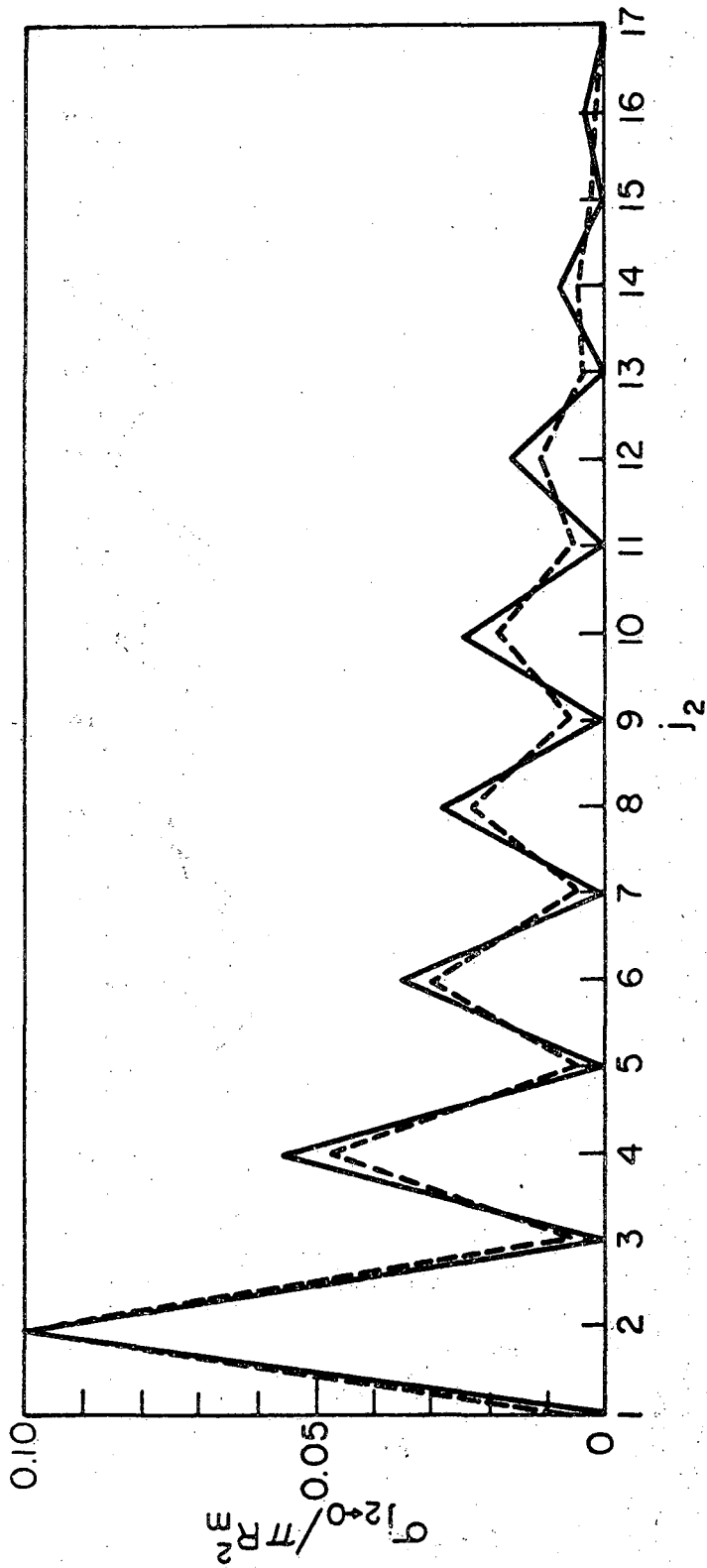
Figure Captions

1. The final rotational quantum number as a function of the initial phase of the rotor. The potential function is that in Eq. (3.6), and the orbital angular momentum $\ell = 10$. The solid curve corresponds to the homonuclear case $a_1 = 0$, $a_2 = 1.2$; this curve is identical in the intervals $(0, \pi)$ and $(\pi, 2\pi)$. The dotted curve is the "almost homonuclear" case $a_1 = 0.15$, $a_2 = 1.2$. The dashed line indicates the graphical solution for the four roots of the equation $j_2(\bar{q}_1) = 10$.
2. Cross sections for rotationally inelastic transitions $j_1 = 0 \rightarrow j_2$. The potential function is given in Eq. (3.6). The solid line connects values for the homonuclear case $a_1 = 0$, $a_2 = 1.2$, and the dashed line the values for the "almost homonuclear" case $a_1 = 0.15$, $a_2 = 1.2$.
3. Same as Fig. 2 except the anisotropy parameters are $(a_1, a_2) = (0.3, 1.2)$ (solid line) and $(a_1, a_2) = (0.4, 1.2)$ (dashed line).
4. Same as Fig. 2 except the anisotropy parameters are $(a_1, a_2) = (0.7, 1.2)$ (solid line) and $(a_1, a_2) = (0.8, 1.2)$ (dashed line).
5. Same as Fig. 2 except the anisotropy parameters are $(a_1, a_2) = (1.0, 0.5)$.



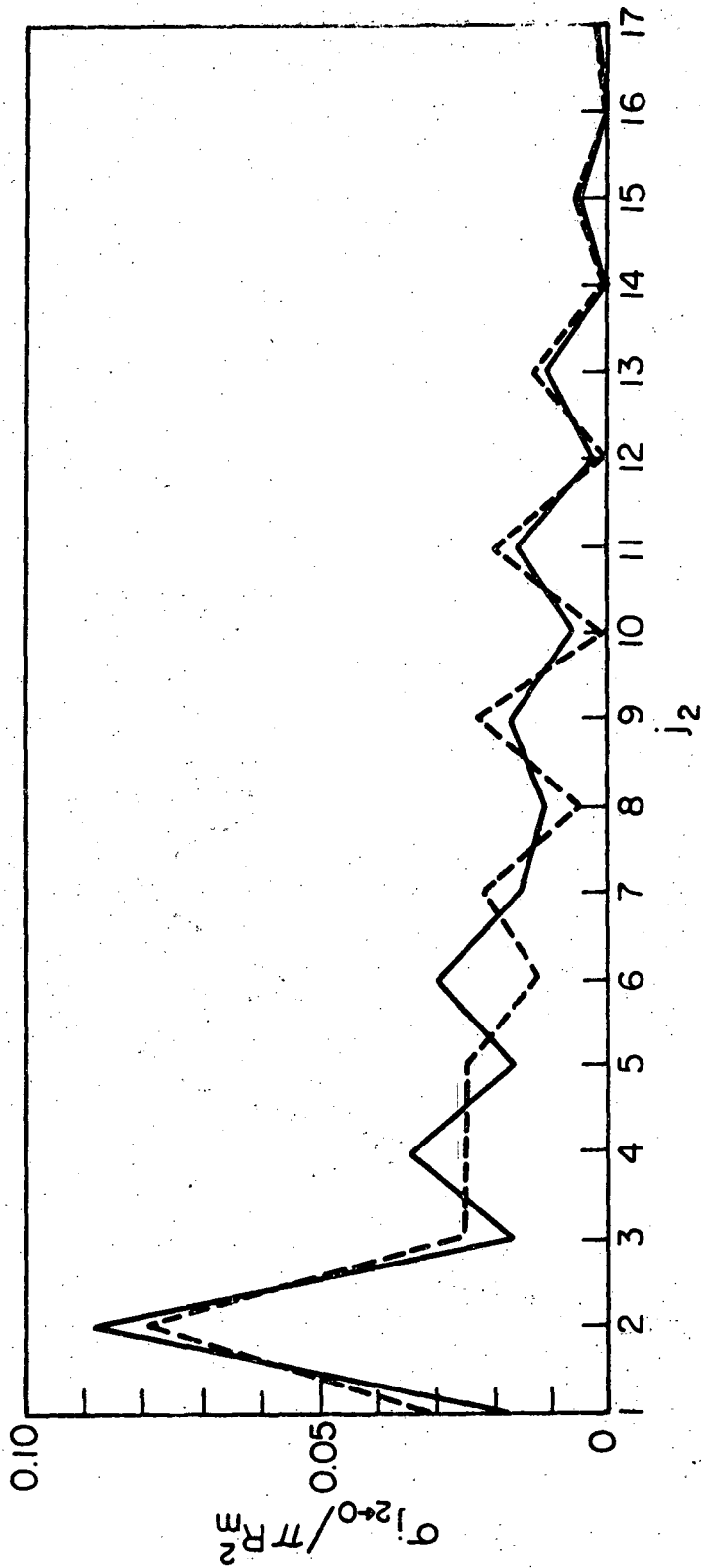
XBL 773-5180

Fig. 1



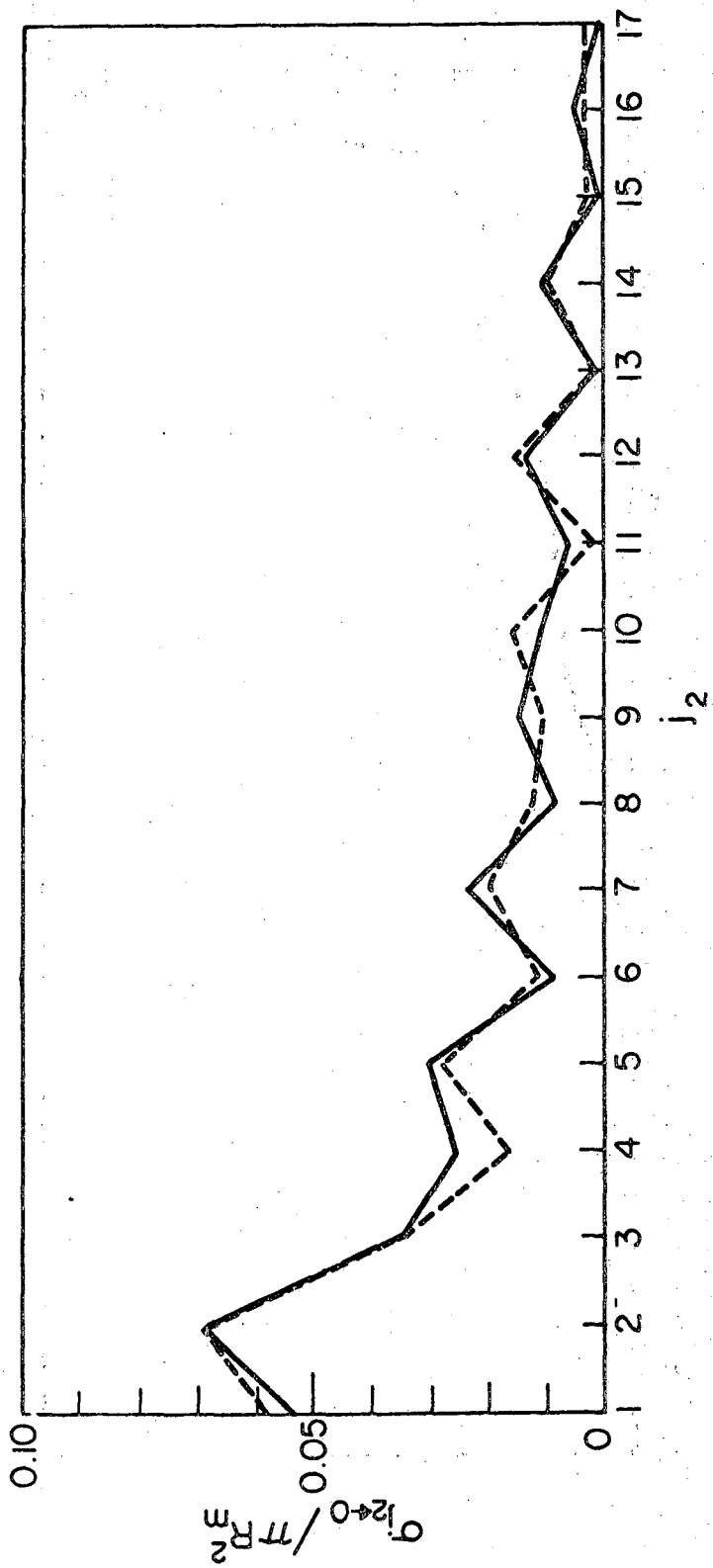
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Fig. 2



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Fig. 3



XBL 773-5183

Fig. 4

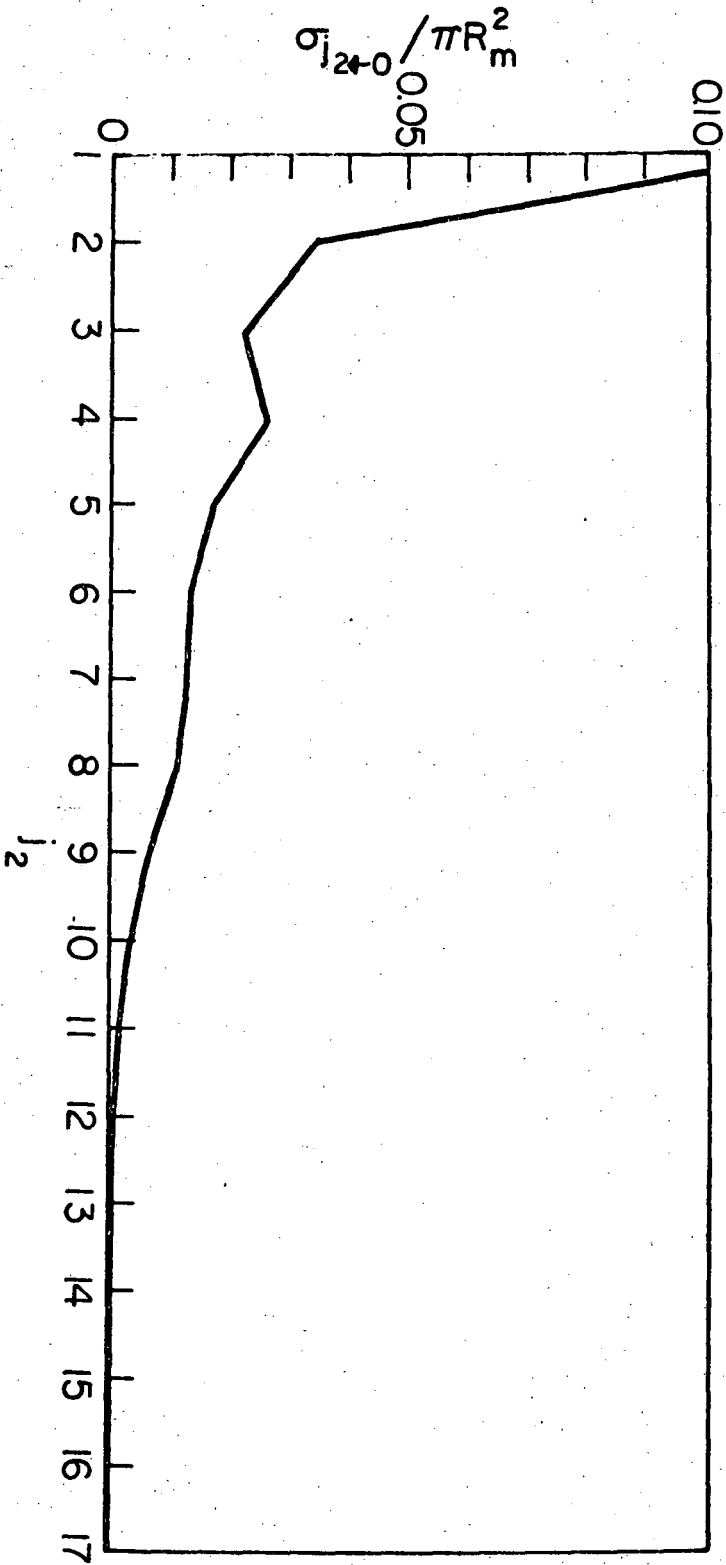


Fig. 5

XBL 773-5184

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