# Geometric phase observed in molecular nitrogen ion.

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**Synopsis** Evidence of a geometric phase is interpreted from non-zero Stokes parameters of the 391.4 nm photon from the X $^2S_g$ molecular ion of nitrogen excited by spin-polarised electrons.

Quantum phenomena pervade the boundaries of space, time and matter. Deformations of oriented shapes, even with zero angular momentum, can be described using gauge potentials and geometric phases [1]. Such effects become observable using the increasing technical capabilities of scientific instrumentations and a realisation that new knowledge comes from measurements after significant reduction of the noise level in instrumentation. Examples exist in polarisation optics, anomalous Hall effect, nuclear magnetic resonance, topological insulators, graphene and molecules [1]

Our work here seeks the presence of a geometric phase in a nitrogen molecule using our optimized spectro-polarimetric approach. Photons, emitted from a state excited by spin-polarised electrons, are observed by their intensity and three Stokes components of the polarisation vector [2[. A non-zero alignment parameter $P_2$ near threshold for excitation was interpreted to identify a geometric phase [2].

This study was inspired by Mead and Truhlar [3] and subsequent treatments of molecular curve crossing Jahn-Teller effects when the potential energy curves involve a spin sign change of the electronic wave functions and associated gauge potential (with geometric path) indicate an effective local magnetic flux. There the evolution of an effective spin-orbit interaction occurs and electron exchange, leads to a geometric phase after a circular transport around a relatively slow moving (nuclear) region. Supporting evidence for theory [3] was given by experiments [4]. Other molecules with Jahn-Teller effects, in which a symmetry plane enables non-adiabatic processes with electronic and nuclear coupling, show orientation and a geometric phase [5] and suggest polarimetry studies.

Interest in molecular nitrogen was attracted by studies [6] of excitation from the neutral ground state X $^1\Sigma_g^+$ (v=0) to the C $^3\Pi_u$ (v'=0) state with photon emission from $B^3\Pi_g$ (v''= 0) + γ (~337 nm) and the $B^3\Pi_g$ (v'' = 2) ni + γ (~380.5 nm) states with observed Stokes parameter $P_2$ equal to zero and implying zero spin-orbit interaction. In contrast to the neutral molecular states, it was shown that excitation to the ion state B $^2\Sigma u^+$ (v' = 0) and its emission to the X $^2\Sigma_g^+$ (v''=0) + γ(~391.4 nm) (P-branch ΔJ=-1) revealed non-zero orientation $P_3$ via spin exchange and non-zero alignment $P_2$ [6]. The non-zero values were attributed to spin exchange, even in the absence of direct spin-orbit coupling, with magnetic coupling of the electron spin with nuclear rotation directly, and with its own residual orbital angular momentum perpendicular to the internuclear axis.

The paradigm of the Born-Oppenheimer approximation and its use by Mead [7] suggest a circular electronic path and geometric phase for the ion excitation. Our measurements indicate nonzero values of the Stokes parameters $P_2$ and $P_3$, and confirm the measurements of [6], but with slightly different values of $P_2$ and $P_3$. We interpret earlier [6] and present data as evidence of a geometric phase.

The need remains for scattering theory to include a geometric phase associated with the structural evolution of a quantum state in addition to the particular Hamiltonian describing the dynamical phase [8].

References

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