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Srisairam Achuthan* (sachutha@math.fsu.edu), 1701,West Pensacola Street, Apt # 202, Tallahassee, FL 32304, and Jack Quine, Tom Asbury and Richard Bertram. Protein Structure Determination by Analysis of Orientational Restraints obtained from Solid State Nuclear Magnetic Resonance. Preliminary report.

Solid state Nuclear Magnetic Resonance gives a method for seeing the shape of proteins from signals given by atoms with spin in the molecule. The signal gives information on the orientation of parts of the molecule with respect to the magnetic field direction \mathbf{B}_0 . Analysis of this information leads to different mathematical problems. First, the molecule must be pieced together from the orientation of its parts. Secondly, the orientations are obtained by solving pairs of quadratic equations, leading to degenerate solutions for \mathbf{B}_0 in a local frame. Finally, the solution depends on the data with various degrees of accuracy. Most of the analysis depends on geometric and differential geometric tools. We give a short discussion of some of these problems. (Received October 04, 2004)