Thermal Motion Analysis via Modern Probability Methods

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Interesting statistical theory advances with crystallographic application possibilities continue to appear. Examples follow:

The Gram-Charlier anharmonic atom model might be replaced by a saddlepoint expansion[1] or a mixture of linear & angular Gaussians.

The refinement matrix from a structure-factor equation in logarithmic form contains a Fisher information matrix[2] with geometric information about interatomic motion coupling.

A stationary Levy stochastic process[3] along a crystal chemistry interaction network may allow atomic displacement models with Levy-jump intramolecular components and Levy-drift intermolecular rigid-body-motion components.

Spatial point processes,[4] e.g. the familiar Gibbs process, allow attraction/avoidance calculation for point particle systems. More general marked point process[4] network node systems with thermal ellipsoid pair Radon-Nikodym derivative[5] couplings seem feasible.

Feasibility studies for a subset of the examples will be discussed.

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[1] Jensen J.L., *Saddlepoint Approximations*, Oxford, 1995. [2] Amari S.I., Nagaoka H., *Methods of Information Geometry*, Oxford, 2000. [3] Sato K.I., *Levy Processes and Infinitely Divisible Distributions*, Cambridge, 1999 [4]. Daley D.J., Vere-Jones D., *Introduction to the Theory of Point Processes, Volume I*, Springer, 2003. [5] Johnson C.K., "Crystallographic Topology 2: Overview and work in progress", *Trends in Mathematical Physics,* Alexiades, V., Siopsis, G. Eds, AMS/IP, 1999.

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