A Matrix Operator Formulation of the Phase Retrieval Problem in Crystallography

Peter Rez (Peter.Rez@ASU.EDU)
Department of Physics and Astronomy and Center for Solid State Science
Arizona State University
Tempe AZ 85287-1504

Fienup has shown that phases can be retrieved from experimentally measured amplitudes provided that the object is embedded in a support region of sufficient size. To recover the phases he used a variant of the Gerchberg-Saxton algorithm that iterated between real and reciprocal space. There are twice as many unknowns as equations in the classic formulation of the phase problem for crystals. It is well understood that embedding in a support region makes the problem determinate, in that the number of equations is either greater to or at least equal to the number of unknowns. For a purely real object the fourier decomposition is best expressed as a sine and cosine series. A matrix formulation shows that the only remaining ambiguity is the sign of the ratio of equivalent coefficients in the sine and cosine series. This should come as no surprise since the problem has been reformulated as a quadratic equation. Although matrix operators might be useful for understanding the formal properties of a solution, they do not necessarily provide an efficient numerical procedure. Practical algorithms can only be devised by analysing competing numerical methods.

J.R. Fienup,J. Opt. Soc. Am. A 4 (1987) 118-123
R.W. Gerchberg and W.O. Saxton, Optik 35 (1972) 237-246