PS02.03.09 UNIQUE PHASE PROBLEM SOLUTIONS FROM REDUCED DENSITY MATRICES: ARE THEY CORRECT? Douglas M. Collins*, Laboratory for the Structure of Matter, 6030 Naval Research Laboratory, Washington DC 20375-5341. Permanent address: Geo-Centers, Inc., 10903 Indian Head Highway, Fort Washington MD 20744

The general phase problem is solved uniquely in a quantum mechanical formulation constructed to display explicitly the main idea of the Hohenberg-Kohn theorem (HKT) ([1964] Phys. Rev. 136, B864-B871). An informal summary of HKT is that electron density alone suffices to delimit fully the ground state of a nondegenerate electronic system. Our focus is on a quantum mechanical representation from which the dependence on spin and all the electrons but one has been removed by integration. Such a representation is a one-particle reduced density matrix (ODM). The fundamental requirement of N-representability is satisfied with the necessary and sufficient condition on ODM eigenvalues that they all lie in the closed interval [0,1] and sum to N, the number of electrons; the admissible ODM set is convex. HKT requires there be an admissible ODM reconstruction from density. Entropy (a function of eigenvalues only) on an ODM is a concave functional, hence entropy’s one and only stationary point is at its global maximum where the eigenvalues are stationary in the parameters of reconstruction, and the corresponding ODM is uniquely determined. Thus maximization of entropy on an admissible ODM necessarily yields a unique solution to the phase problem.

Is the solution correct if structure moduli are known but phases are variables of the reconstruction? Clearly, if two or more structures have identical structure moduli, only by chance can a direct method select a particular result, but this is a most improbable situation. Can this method generate a reasonable and well-behaved representation of this new theory on the fundamental requirement of N-representability is satisfied with the necessary and sufficient condition on ODM eigenvalues that they all lie in the closed interval [0,1] and sum to N, the number of electrons; the admissible ODM set is convex. HKT requires there be an admissible ODM reconstruction from density. Entropy (a function of eigenvalues only) on an ODM is a concave functional, hence entropy’s one and only stationary point is at its global maximum where the eigenvalues are stationary in the parameters of reconstruction, and the corresponding ODM is uniquely determined. Thus maximization of entropy on an admissible ODM necessarily yields a unique solution to the phase problem.

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PS02.03.10 INTEGRATED DIRECT METHOD WITH ANOMALOUS SCATTERING: TRIPLETS - SECOND NEIGHBOURHOOD. D. Velmurugan and D. Subbhashini, Department of Crystallography and Biophysics, University of Madras, Madras - 600 025, India

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