N-representable one-electron reduced density matrices reconstruction at non-zero temperatures.

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This work retraces different methods that have been explored to account for the atomic thermal motion in the reconstruction of one-electron reduced density matrices from experimental X-ray structure factors (XSF) and directional Compton profiles (DCP). Attention has been paid to propose the simplest possible model, which obeys the necessary N-representability conditions, while accurately reproducing all available experimental data.

The deconvolution of thermal effects makes it possible to obtain an experimental static density matrix, which can directly be compared with theoretical 1-RDM. It is found that above a 1% statistical noise, the role played by Compton scattering data becomes negligible and no accurate 1-RDM becomes reachable.

Since no thermal 1-RDM is available as a reference, the quality of an experimentally derived temperature-dependent matrix is difficult to assess. However, the accuracy of the obtained static 1-RDM is strong evidence that the Semi-Definite Programming method is robust and well-adapted to the reconstruction of an experimental dynamical 1-RDM.

Keywords: Density matrices; Temperature smearing; Compton scattering; X-Ray diffraction.

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