Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Method for the Direct Solve of the Many-Body Schrödinger Wave Equation[1] JONATHAN JERKE, Texas Tech University, C. J. TYMCZAK, Texas Southern University, BILL POIRIER, Texas Tech University — We report on theoretical and computational developments towards a computationally efficient direct solve of the many-body Schrödinger wave equation for electronic systems. This methodology relies on two recent developments pioneered by the authors: 1) the development of a Cardinal Sine basis for electronic structure calculations [arXiv:1405.5073; Jerke, JCP 2015 143]; and 2) the development of a highly efficient and compact representation of multidimensional functions using the Canonical tensor rank representation developed by Belykin et. al. [SIAM 2005 26(6)] which we have adapted to electronic structure problems. We then show several relevant examples of the utility and accuracy of this methodology, scaling with system size, and relevant convergence issues of the methodology.

[1]Method for the Direct Solve of the Many-Body Schrdinger Wave Equation

C. J. Tymczak
Texas Southern University

Date submitted: 14 Nov 2016 Electronic form version 1.4