Abstract Submitted
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Numerical Interpolation of Orbitals in Periodic Systems for Diffusion Monte Carlo Calculations WILLIAM PARKER[1], KEVIN DRIVER, PHILLIP PETERSON, RICHARD HENNIG, JOHN WILKINS, Ohio State University, CYRUS UMRIGAR[2], Cornell University — Diffusion Monte Carlo methods provide accurate energies for complex materials, however, the algorithms are computationally intensive. Representing the orbitals of the Slater determinant numerically with splines reduces the time scaling from O(N^3) to O(N^2) [3]. We compare memory and time requirements and the accuracy dependence on the number of grid points for cubic spline and Lagrange interpolation schemes in periodic systems. Both interpolation schemes have a small prefactor, providing speedup even for small systems. For example, in bulk silicon with 256 electrons, Lagrange interpolation reduces the computation time by a factor of 70. We are currently working on the implementation of different splines routines.

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[2]Support from NSF and Sandia National Laboratories
[3]A. J. Williamson, R. Q. Hood, and J. C. Grossman. PRL **87**, 246406 (2001).

William Parker
Ohio State University

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