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Efficient orbital storage and evaluation for quantum Monte Carlo simulations of solids KENNETH ESLER, Carnegie Institution of Washington — Researchers have applied continuum quantum Monte Carlo methods to solids with great success, but thus far applications have been largely limited to crystals with simple geometry. In these simulations, three-dimensional cubic B-splines have proven to be a fast and accurate means of storing and evaluating electron orbitals. While B-splines require less memory than other spline interpolation schemes, modern cluster nodes often have insufficient memory to store the orbitals for more complex systems. We introduce three techniques, appropriate in different circumstances, to dramatically reduce the memory required for orbital storage, while retaining high accuracy: the generalized tiling of primitive-cell orbitals into a supercell of arbitrary shape, the use of nonuniform grids for localized orbitals, and the periodic replication of localized orbitals. We give examples for cubic boron nitride and wüstite (FeO), and show that these methods can reduce the memory used for orbital storage by more than two orders of magnitude. Finally, we introduce an open-source B-spline library to facilitate the incorporation of these methods into QMC simulation codes.

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