

Abstract Submitted
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Interfacing Determinant Quantum Monte Carlo and Density Functional Theory¹ NIKOLAI ZARKEVICH, University of California, Davis, CA 95616, ZHAOJUN BAI, Computer Science Department, University of California, Davis, CA 95616, SERGEY SAVRASOV, RICHARD SCALETTAR, Physics Department, University of California, Davis, CA 95616, MARK JARRELL, Physics Department, University of Cincinnati, OH 45221 — Over the last decade many body theory and electronic structure calculations have come together within the “LDA+DMFT” approach in which dynamical mean field theory (DMFT) provides a frequency dependent self-energy $\Sigma(\omega)$ for electronic structure calculation within the local density approximation (LDA). Here we describe initial results with a new approach which uses the determinant Quantum Monte Carlo method to supply the self energy. This technique has the advantage of providing a momentum dependent $\Sigma(\mathbf{k}, \omega)$. However, the fermion sign problem can limit the ability to access the ground state value of the self energy. We present tests of the approach on a model of cuprate superconductors.

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