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Compact representation of the Green function of an infinite periodic system JONATHAN E. MOUSSA, MARVIN L. COHEN, University of California at Berkeley and Lawrence Berkeley National Laboratory — The single particle Green function of a periodic system is typically constructed by first calculating the band structure of the system and then summing up wavefunctions and energy denominators in the usual way. To construct an accurate Green function, many unoccupied bands must be included and k-points have to be sampled carefully, making use of both symmetries and approximate integration techniques. An alternate form of the Green function is presented, not based on band structures but rather local coordinate transformations. This method makes no use of Bloch's Theorem and instead exploits periodicity using renormalization-like scaling ideas. Calculations are performed with a localized basis set and the cost is demonstrated to be proportional to the log of the number of included unit cells and linearly scaling with unit cell size.

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