

Development of a Fock Exchange Calculation Method for Twisted Bilayer Graphene Based on Interpolative Decomposition and FFT

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Twisted bilayer graphene (TBG), two graphene layers stacked with a small relative rotation, hosts strongly correlated phases such as superconductivity, Mott insulating states, and the quantum anomalous Hall effect, depending on the twist angle. Describing their band structure, topology, and gaps accurately requires treating the nonlocal Fock exchange in mean-field calculations [1], which is computationally demanding. In TBG, a unit cell contains thousands to tens of thousands of atoms, the internal degrees of freedom are numerous, and the momentum integral requires a dense grid. Previous studies have therefore retained only the components with equal reciprocal lattice vectors [1].

We are developing a method combining the interpolative decomposition (ID) [2], a low-rank matrix approximation, with the fast Fourier transform (FFT) [3] to compute the Fock exchange including the components with different reciprocal lattice vectors. The density matrix, with the internal degrees of freedom as rows and the momentum as columns, has several thousand rows expected to be largely linearly dependent. The ID selects representative rows and approximates the rest by their linear combinations, and only the selected rows are convolved with the Coulomb interaction by FFT on the momentum grid.

We have implemented the Fock exchange matrix for a single self-consistent step and confirmed that the number of selected rows saturates as the number of reciprocal lattice vectors increases, remaining at a few percent of the total, while the error is controlled by the ID tolerance. We report the formulation, cost, and accuracy of the method and discuss its incorporation into self-consistent calculations.

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