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Symmetry-Checking in Band Structure Calculations on a Noisy Quantum Computer

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Band crossings in electronic band structures play an important role in determining the electronic, topological, and transport properties in solid-state systems, making them central to both condensed matter physics and materials science. The emergence of noisy intermediate-scale quantum (NISQ) processors has sparked great interest in developing quantum algorithms to compute band structure properties of materials. While significant research has been reported on computing ground state and excited state energy bands in the presence of noise that breaks the degeneracy, identifying the symmetry at crossing points using quantum computers is still an open question. In this work, we propose a method for identifying the symmetry of bands around crossings and anti-crossings in the band structure of bilayer graphene with two distinct configurations on a NISQ device. The method utilizes eigenstates at neighbouring **k** points on either side of the touching point to recover the local symmetry by implementing a character-checking quantum circuit that uses ancilla qubit measurements for a probabilistic test. We then evaluate the performance of our method under a depolarizing noise model, using four distinct matrix representations of symmetry operations to assess its robustness. Finally, we demonstrate the reliability of our method by correctly identifying the correct band crossings of AA-stacked bilayer graphene around K point, using the character-checking circuit implemented on a noisy IBM quantum processor $ibm\_marrakesh$.

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