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Quantum Monte Carlo Simulations in Momentum Space

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Quantum Monte Carlo (QMC) methods are powerful numerical tools that can simulate quantum many-body problems with strong interactions among particles. Among them, determinant QMC is the most popular scheme which usually deals with the interacting fermions on a finite lattice system, such as the Hubbard model, Heisenberg model and periodical Anderson model. The key step of determinant QMC is to express the partition function that determines the thermal dynamical properties to a summation of terms with each of them being a "determinant" obtained by solving a corresponding non-interacting fermion model characterized by a set of Bosonic fields resulted from the "Hubbard–Stratonovich" transformation and Trotter decomposition.[1] Therefore, the determinant QMC maps a quantum many-body problem to a classical statistical problem if the determinant mentioned above is always positive and can be explained as some kind of probability. With the help of importance sampling and Metropolis process, the summation for the partition function can then be performed by considering random walk of the above Bosonic fields in the configuration space. Due to its simplicity, determinant QMC has been widely applied to various lattice Fermion models with strong local interactions as an unbiased way to conduct "numerical experiments". The main problem that prevents the determinant QMC to achieve further success is the so-called "sign problem", which is commonly encountered in many quantum many-body problems. The sign problem comes from the fact that the determinant associated with the each configuration is not always positive, which heavily reduces the efficiency of the importance sampling. The sign problem usually gets worse very quickly with the decrement of the temperature, which prevents the determinant QMC to be applied to enough low temperature, where the "quantumness" of the problem is about to fully emerged. Therefore, quantum systems with no or mild sign problems become very interesting because these problems can be efficiently studied by the QMC method, which allows us to take the full advantage of "Moore's law".

Usually the property of no sign problem is not universal for all possible representations of the model. In most of the cases, it is only true for some special single particle basis set, where the smartly chosen way of rearranging the partition function guarantees that all the determinants involved have the same sign as a consequence of some unique symmetries. Recently, for a very important quantum many-body problem, the twisted bi-layer graphene systems,[2,3] Meng's group from Hong Kong University developed a completely new QMC scheme,[4] which works in momentum space instead of the real space to avoid the sign problem. Unlike the lattice Fermion models in the traditional strong correlated systems, the interacting electrons in TBG are more convenient to be described in the momentum space due to the following two reasons. First, the single particle wave functions, which are the basis of the correlation problems, extend as wide as several tens of lattice constants. Second, the effective interaction among those electrons near the Fermi level cannot be described as Hubbard-like short range interactions. Instead, it is the finite range screened Coulomb potential, which also covers tens of lattice constants. Professor ZiYang Meng and his collaborators revealed that the QMC scheme in momentum space provides a much natural description for the TBG systems and can have sign problem free for several different situations, which allows quite precise numerical simulation for this interesting new quantum many-body problem. The first round results from this new method on TBG were published in Ref. [4], which convincingly demonstrated the validity of the method by comparing with the exact solutions for some benchmark cases.[5] Considering the fact that new strongly correlated systems in 2D materials keep appearing in recent years, the new QMC method in momentum space developed by Meng's group will become more and more useful for future studies of related systems.

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