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Research statement
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My primary research interests are model design and numerical investigations using quantum Monte Carlo (QMC) method, to study quantum criticality, non-Fermi liquid (nFL) and quantum moiré models. I'm also interested in algorithms developments and Sign Problem in QMC simulation. More broadly, running through all of my research are three major topics which shape and direct my efforts:

- The theory of quantum criticality, especially for the itinerant electrons, which is of great help in describing the behaviors of non-Fermi liquid(nFL)[1, 2, 3, 4] and exotic transport properties near quantum critical points(QCPs). The famous Hertz-Millis-Moriya(HMM) theory has a rich history, while research beyond it is even more fascinating.
- The twistronics in Quantum Moiré systems such as twisted bilayer graphene (TBG)[5, 6, 7, 8] and twisted metal transition metal dichalcogenides (TMD)[9], which exhibit rich phase diagram of correlated insulating and superconducting phases thanks to the high tunability by twisting angles, gating and tailored design of the dielectric environment, brings new vitality to the field of strongly correlated electronic systems.
- The development of QMC computational methods, such as the development of update algorithms [10], new understanding of the notorious sign problem[11, 12] and the model design[2, 3, 6, 13, 14] for computation with no sign problem or algebraic decay sign problems.

In what follows, I describe several current areas of my research.

Quantum criticality and nFL behaviors

In the study of correlated materials, quantum criticality in itinerant electron systems is of great importance and interests . It plays a vital role in the understanding of anomalous transport, strange metal and nFL behaviors in the vicinity of QCPs of heavy-fermion materials, Cu- and Fe-based high-temperature superconductors, and transition-metal alloys. These novel properties, which do not fitted into traditional quantum many-body paradigms such as the Fermi liquid theory of metals and the Landau-Ginzburg-Wilson framework, caught my interest.

Spin-fermion coupled model:

In a general context, nFL behavior often occurs via electron interactions mediated by gapless bosonic modes that render the electrons incoherent. Such gapless bosons typically arise in the vicinity of a QCP or in quantum gauge theories.

We designed a spin-fermion coupled square lattice model[1, 2], which has an itinerant QCP with fermion pockets and hot spots, and developed quantum Monte Carlo simulation to examine itinerant QCPs generated by antiferromagnetic fluctuations. Then we unambiguously reveal the nFL fermion self-energy and the bosonic dynamic susceptibilities.

Near the AFM-QCP, fermions at the hot spots shows non-Fermi liquid behavior. The The Matsubara-frequency dependence of the $\mathrm{Im}(\Sigma(k,\omega))$ goes to a small constant at low ω, and no sign of either linear vanishing or diverging are observed. The not a small anomalous dimension $\eta = 0.25$ we detected is significantly different from the Hertz-Millis theory prediction.

Self-tune spin-1/2 Yukawa-SYK model:

In addition, since it is very difficult to tune the system to the quantum critical region. The precise determination of the quantum critical point and region of nFL are subject to finite size effects, and the position of the QCP is not universal but system dependent. We also turn to study the self-tuned Yukawa-SYK model[3, 4].

Unlike the itinerant QCP models where the systems live in 2 spatial dimensions, the Yukawa-SYK models live in infinite dimensions and have been shown to "self-tune" to quantum criticality within large-N approximation. Here self-tuned means the system is critical, independent of the bosonic bare mass m_0, which gives us a large area of nFL.

We performed unbiased sign-problem free quantum Monte Carlo simulations of the Yukawa-SYK model, and reported direct evidence of self-tuned quantum-critical and nFL behaviors of Green functions, which have the form $G_f(\tau,0) \propto \left(\frac{\pi}{\beta\sin(\pi\tau/\beta)}\right)^{1-x}$ and $G_b(\tau,0) \propto \left(\frac{\pi}{\beta\sin(\pi\tau/\beta)}\right)^{2x}$.

Quantum Monte Carlo simulations for Twisted Systems

Quantum Moiré systems such as TBG and twisted TMD systems, bestowed with the quantum geometry of wavefunctions – manifested in the distribution of Berry curvature in the flat bands – and strong long-range Coulomb electron interactions, exhibit rich phase diagram of correlated insulating and superconducting phases thanks to the high tunability by twisting angles, gating and tailored design of the dielectric environment. The extremely active research field of 2D quantum Moiré materials is developing very fast.

Momentum-space models and quantum Monte Carlo method:

We start from the continuous Bistritzer-MacDonald(BM) model and long range single-gate Coulomb interaction, and integrate out the states on the remote bands to obtain the projected Hamiltonian, which has considered the long-range Coulomb interaction and the Wannier obstruction problem. The momentum-space method [5] we developed is free of the sign problem at charge-neutrality point(CNP) with the C_2P and C_2T symmetries. For other integer filling, there are sign problems in general, but we can also discussed the computational possibilities[6].

TBG:

Since we developed the momentum-space QMC method for twisted system. We compute the spectra of both single-particle and particle-hole excitations. We found that at CNP [7], the intervalley coherent(IVC) state is the leading instability, with strong competition from the valley polarized (VP) state. In addition, at low-energy, longlived valley waves are observed in close analogy to spin waves of a Heisenberg ferromagnet, while these modes become over-damped as their energy reaches the particle-hole continuum.

And in the chiral limit and flat band limit, it is fortunate enough for us to be able to study the physics of $\nu = 1$ [8], although there is a sign problem now. In the low temperature limit, the sign of this system converges to a finite value and decays algebraically rather than exponentially with system size L. This allows us to perform QMC simulations. The Ising thermal transition and the QAH-TMI state which emerges at $T = 0$ are observed. The transition temperature T_c is dramatically smaller than the energy scale of the gap at zero temperature. And we show that it's caused by excitonic excitations in the particle-hole channel.

Inter-valley attractions and twisted TMD:

We show that by matching the interaction strength of inter-valley attraction with intra-valley repulsion, the flat-band limit becomes exactly solvable. Away from the flat-band limit, the system can be simulated via QMC methods without sign problem for any fillings. As an example, we reveal nontrivial phenomena in twisted TMD[9], such as doping independent gap and large compressibility above the superconducting dome.

Quantum Monte Carlo methods

As mentioned earlier, we designed a lot of models[1, 2, 3, 4, 5, 7, 13, 14] without sign problem to conduct different studies. At the same time, we have also carried out some tests[10] for different QMC update algorithms.

In addition, in order to deepen our understanding of the sign problem in QMC[11, 12], especially the fermion sign problem, we develop the Sign Bound Theory.

Sign Problem in QMC and Sign Bound Theory:

Usually, if there is a sign problem, the average of sign usually decays exponentially to zero with inverse of temperature β and system size L. However, in some systems, we find that in the zero temperature limit, the sign does not decay exponentially with respect to system size L but rather decay algebraically.

In fact, in the zero temperature limit, the mean of the signs is related to the ground state energy and ground state degeneracy of the original system and the reference system. When we choose a good reference system, the two ground state energys are equal, and the sign is just a function of the degeneracy of the two systems. Our Sign Bound Theory[12] discusses the relevant details and attempts to give an upper bound on the degeneracy of the reference system in some cases, which leads to a lower bound on the sign.

The theory guides us to QMC simulations of some twisted systems[6, 8] with sign problem. In these cases, although there is a sign problem, the average of sign has a polynomial lower bound with respect to system size L in the zero temperature limit, so the simulation can be carried out at an acceptable cost.

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