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Overcoming Fermionic Sign Problem in Lattice Quantum Monte Carlo: A Cuprate Case

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We developed a strong coupling perturbation scheme for general Hubbard model around half-field particle-hole symmetric reference system [1]. The approach based on a lattice determinatal Quantum Monte Carlo method in continuous and discrete time versions [2] for a large periodic clusters in a fermionic bath. The first and second order perturbation in the shift of chemical potential and long-range hopping gives a reasonable accuracy for parameters corresponding to the optimal cuprate systems. We calculate spectral function of doped t-t'-U model for interaction strength equal to the band width and discuss a mechanism of the pseudogap formation. Results for standard cuprates model with $U=8t=W$ and $t'/t=-0.3$ for the temperature of the order of $T=0.1t$ show formation of the Fermi-arcs. We discuss the magnetic and superconducting instability using symmetry broken external fields.

[1] S. Iskakov, M. I. Katsnelson, A. I. Lichtenstein, npj Comp. Materials 10, 36 (2024).
[2] E. Gull, A. J. Millis, A. I. Lichtenstein, et. al., Rev. Mod. Phys. 83, 349 (2011).

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