Antiferromagnetism and Superconductivity in Dual-Fermion Lattice Quantum Monte Carlo

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Abstract

We investigate response of the correlated lattice model on external magnetic or superconducting field. The approach is based on the lattice determinantal Quantum Monte Carlo (QMC) method in continuous and discrete time versions for large periodic clusters in a fermionic bath. Considering the first-order perturbation in the shift of the chemical potential and of the second-neighbour hopping gives an accurate electronic spectral function for a parameter range corresponding to the optimally doped cuprate system for temperature of the order of $T = 0.1t$, the region hardly accessible for the straightforward lattice QMC calculations. We discuss the antiferromagnetism and superconductivity for a doped Hubbard system in a strong-coupling regime with the interaction parameter U equal to the bandwidth and the optimal value of the next-nearest-neighbor hopping parameter t' for high-temperature superconducting cuprates.

INTRODUCTION

Search for numerically exact solution of the $t - t' - U$ Hubbard model in thermodynamic limit at arbitrary interaction strength, long-range hoppings and doping δ or, equivalently, chemical potential μ at low temperature $T = 1/\beta$ is tremendously difficult.

RESULTS

DISCUSSION

METHODS

We start with the general version of the cluster or multi-orbital dual fermion scheme for $t-t'-U$ square lattice Hubbard model. The dual fermion approach as a strong coupling theory is related to formally exact expansion around arbitrary reference system

Hamiltonian

The simplest model describing interacting fermions in the external AFM or Dw fields on a lattice is the single band Hubbard model, defined by the Hamiltonian

$$\hat{H}_\alpha = -\sum_{i,j,\sigma} t_{ij}^{\alpha} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_i U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) + \alpha h_{ext} \tag{1}$$

where t_{ij} is the hopping matrix elements including the chemical potential μ in the diagonal elements.

$$t_{ij}^{\alpha} = \begin{cases} t & \text{if } i \text{ and } j \text{ are nearest neighbours,} \\ \alpha t' & \text{if } i \text{ and } j \text{ are next nearest neighbours,} \\ \alpha\mu & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases} \tag{2}$$

where $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. We introduce a "scailing" parameter $\alpha = 0, 1$, which defined a reference system H_0 for $\alpha = 0$ which corresponds to the half-filled Hubbard model ($\mu_0 = 0$) with only nearest neighbours hoppings ($t'_0 = 0$) and final system H_1 for $\alpha = 1$ for given μ and t' and AFM or Dw fields h_{ext}. Notes, that long-range hoping parameters can be trivially included similar to t'.

Real space scheme

For the super-perturbation in the lattice Monte-Carlo scheme we use a general dual-fermion expansion around arbitrary reference system within the path-integral formalism [**?**, **?**] similar to a strong coupling expansion [**?**]. In this case our $N \times N$ lattice and corresponding reference systems represent $N \times N$-part which we cut from infinite lattice and periodise the bare Green's function $\mathcal{G}_\alpha$ (see Supplementary Note 1). The general lattice action for discretise $N \times N \times L$ space-time lattice (for CT-INT scheme imaginary time space τ is continuous in the $[0, \beta)$ interval) with Hamiltonian Eq. (1) reads

$$S_\alpha[c^*, c] = -\sum_{1,2} c_1^* \, (\mathcal{G}_\alpha)_{12}^{-1} \, c_2 + \frac{1}{4} \sum_{1234} U_{1234} c_1^* c_2^* c_4 c_3 \, . \tag{3}$$

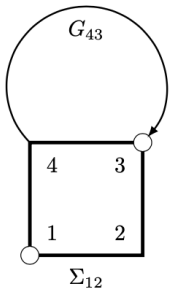

Figure 1: Feynman diagram for the first order dual fermion perturbation for the self-energy $\tilde{\Sigma}_{12}$: a line represents the non-local dual Green's function $\tilde{G}_{43}$ and a box is the two-particle vertex γ_{1234}.

In order to keep the notation simple, it is useful to introduce the combined index $|1\rangle \equiv |i, \tau, \sigma\rangle$ (i being the site index suppressed above) while assuming summation over repeated indices.

To calculate the bare propagators $(\mathcal{G}_\alpha)_{12}$ we start from the $N \times N$ cluster which is cut from infinite lattice and then force translation symmetry and periodic boundary condition on the finite $N \times N$ system. This procedure is easy to realize in the k-space, by doing first a double Fourier transform of the bare Green's function for non-periodic $N \times N$ cluster $\mathcal{G}^{\alpha}_{\mathbf{k},\mathbf{k}'}$ and then keep only periodic part, $\mathcal{G}^{\alpha}_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}$.

Perturbation matrix of one-electron part of Action:

$$\tilde{t} = \mathcal{G}_0^{-1} - \mathcal{G}_1^{-1}\,. \tag{4}$$

The dual action in paramagnetic state reads

$$\tilde{S}\,[d^*, d] = -\sum_{\mathbf{12}\,\nu\sigma} d^*_{1\nu\sigma}\,(\tilde{G}^0_\nu)^{-1}_{12}\,d_{2\nu\sigma} + \frac{1}{4}\sum_{1234}\gamma_{1234} d^*_1 d^*_2 d_3 d_4, \tag{5}$$

where the bare dual Green's function has the following matrix form:

$$\tilde{G}^0_{12} = \left[\,\tilde{t}^{-1} - \hat{g}\,\right]^{-1}_{12} \tag{6}$$

with g being exact Green's matrix of the interacting referemnce system.

We used the following notation for the four-point vertex:

$$\gamma_{1234} = \langle c_1 c^*_2 c_4 c^*_3\rangle - \langle c_1 c^*_2\rangle\langle c_4 c^*_3\rangle + \langle c_1 c^*_3\rangle\langle c_4 c^*_2\rangle \tag{7}$$

The DF-first order diagram shown in Fig.**??** in particle-hole (PH) channel is given by

$$\tilde{\Sigma}^{(1)}_{12} = -\sum_{s-QMC}\sum_{3,4}\gamma^d_{1234}(s)\tilde{G}^0_{34} \tag{8}$$

Here the density vertex in PH channel is

$$\gamma^{d}_{1234} = \gamma^{\uparrow\uparrow\uparrow\uparrow}_{1234} + \gamma^{\uparrow\uparrow\downarrow\downarrow}_{1234} \tag{9}$$

and the final Green's function reads

$$G_{12} = \left[\left(g + \tilde{\Sigma}\right)^{-1} - \tilde{t}\right]^{-1}_{12} \tag{10}$$

Within the determinant DQMC with Ising-fields $\{s\}$ or inside the CT-INT with stochastic sampling of interaction order expancion $\{s\}$ for two-particle correlators we can use the Wick-theorem:

$$\gamma_{1234}(s) \equiv \langle c_1 c^*_2 c_3 c^*_4\rangle_s = \langle c_1 c^*_2\rangle_s \langle c_3 c^*_4\rangle_s - \langle c_1 c^*_4\rangle_s \langle c_3 c^*_2\rangle_s \tag{11}$$

Within the QMC Markov chain the lattice auxilary Green's function is not translationally invariant therefore $g^s_{12} = -\langle c_1 c^*_2\rangle_s$ and we use double Fourier transform to calculate $g^s_{kk'}$. To include "disconnected part" of the vertex in equation Eq. (7) we just substract exact Green's function from the previus QMC run of the reference system as following

$$\tilde{g}^s_{12} = g^s_{12} - g_{12} \tag{12}$$

With this definition we can rewrite the 1-st order DF-perturbation in the following matrix-spinor form in paramagnetic Reference system:

$$\tilde{\Sigma}^{\uparrow\uparrow}_{12} = -\sum_{3,4}\left[\langle c_{1\uparrow} c^*_{2\uparrow} c_{3\uparrow} c^*_{4\uparrow}\rangle \tilde{G}^{\uparrow\uparrow}_{43} + \langle c_{1\uparrow} c^*_{2\uparrow} c_{3\downarrow} c^*_{4\downarrow}\rangle \tilde{G}^{\downarrow\downarrow}_{43}\right] \tag{13}$$

$$\tilde{\Sigma}^{\downarrow\downarrow}_{12} = -\sum_{3,4}\left[\langle c_{1\downarrow} c^*_{2\downarrow} c_{3\downarrow} c^*_{4\downarrow}\rangle \tilde{G}^{\downarrow\downarrow}_{43} + \langle c_{1\downarrow} c^*_{2\downarrow} c_{3\uparrow} c^*_{4\uparrow}\rangle \tilde{G}^{\uparrow\uparrow}_{43}\right] \tag{14}$$

$$\tilde{\Sigma}^{\uparrow\downarrow}_{12} = -\sum_{3,4}\langle c_{1\uparrow} c^*_{2\downarrow} c_{3\downarrow} c^*_{4\uparrow}\rangle \tilde{G}^{\uparrow\downarrow}_{43} \tag{15}$$

Within the QMC, using the Wick-theorem Eq.(11) we have

$$\tilde{\Sigma}^{\uparrow\uparrow}_{12} = -\sum_{QMC}\sum_{3,4}\left[\left(\tilde{g}^{\uparrow}_{12}\tilde{g}^{\uparrow}_{34} - \tilde{g}^{\uparrow}_{14}\tilde{g}^{\uparrow}_{32}\right)\tilde{G}^{\uparrow\uparrow}_{43} + \tilde{g}^{\uparrow}_{12}\tilde{g}^{\downarrow}_{34}\tilde{G}^{\downarrow\downarrow}_{43}\right] \tag{16}$$

$$\tilde{\Sigma}^{\downarrow\downarrow}_{12} = -\sum_{QMC}\sum_{3,4}\left[\left(\tilde{g}^{\downarrow}_{12}\tilde{g}^{\downarrow}_{34} - \tilde{g}^{\downarrow}_{14}\tilde{g}^{\downarrow}_{32}\right)\tilde{G}^{\downarrow\downarrow}_{43} + \tilde{g}^{\downarrow}_{12}\tilde{g}^{\uparrow}_{34}\tilde{G}^{\uparrow\uparrow}_{43}\right] \tag{17}$$

$$\tilde{\Sigma}^{\uparrow\downarrow}_{12} = +\sum_{QMC}\sum_{3,4}\tilde{g}^{\uparrow}_{14}\tilde{g}^{\downarrow}_{32}\tilde{G}^{\uparrow\downarrow}_{43} \tag{18}$$

and the final Green's function reads

$$G_{12} = \left[\left(g + \tilde{\Sigma}\right)^{-1} - \tilde{t}\right]^{-1}_{12} \tag{19}$$

For small system (see Supplementary Note 2) we can calculate matrix of Green's function from Eq. (19) directly in the real space formalism.

K space scheme

For large system ($N \geq 4$) it is much faster to calculate the dual self-energy in the K-space with within the QMC Markov chain. The dual action in K-space reads

$$\tilde{S}\,[d^*, d] = -\sum_{\mathbf{k}\,\nu\sigma} d^*_{\mathbf{k}\nu\sigma}\; \tilde{G}^{-1}_{0\mathbf{k}\nu}\; d_{\mathbf{k}\nu\sigma} + \frac{1}{4}\sum_{1234} \gamma_{1234} d^*_1 d^*_2 d_3 d_4\,. \tag{20}$$

Using the short notation $k \equiv (\mathbf{k}, \nu_n)$ and $\nu_n = (2n+1)\pi/\beta$, with $n \in \mathbb{Z}$, the dual Green's function is equal to

$$\tilde{G}^0_k = \left(\tilde{t}^{-1}_k - \hat{g}_k\right)^{-1}\,. \tag{21}$$

We discuss now external AFM field with Q=(π,π) or Dw field with (Q=0) which both proportional to σ_x Pauli matrix and acts only for $\alpha = 1$ in Eq.(1) which lead to new "perturbation" matrix of one-electron part of Action:

$$\tilde{t}_k(h_Q) = \mathcal{G}^{-1}_0 - \mathcal{G}(h_Q)^{-1}_1 = \tilde{t}_k + h\,\sigma_x \delta_{k,Q} \tag{22}$$

In the case of AFM external field we have general (complex) the spinor form of perturbation

$$\tilde{t}_k(h_Q) = \begin{pmatrix} \tilde{t}_k & h_Q \\ h^*_Q & \tilde{t}_{k+Q} \end{pmatrix} \tag{23}$$

Therefore the bare Dual Green's function has the following spinor form

$$\tilde{G}^0_k = \left[\begin{pmatrix} \tilde{t}_k & h_Q \\ h^*_Q & \tilde{t}_{k+Q} \end{pmatrix}^{-1} - \begin{pmatrix} g_k & 0 \\ 0 & g_{k+Q} \end{pmatrix}\right]^{-1} \tag{24}$$

For the d-wave HTSC field (Q=0) but k-dependent:

$$\Delta_k = 2h_{dw}(\cos k_x - \cos k_y) \tag{25}$$

with corresponding dual-perturbation

$$\tilde{t}_k(h_{dw}) = \begin{pmatrix} \tilde{t}_k & \Delta_k \\ \Delta^*_k & -\tilde{t}^*_k \end{pmatrix} \tag{26}$$

and HTSC-field bare dual Green's function

$$\tilde{G}^0_k = \left[\begin{pmatrix} \tilde{t}_k & \Delta_k \\ \Delta^*_k & -\tilde{t}^*_k \end{pmatrix}^{-1} - \begin{pmatrix} g_k & 0 \\ 0 & -g^*_k \end{pmatrix}\right]^{-1} \tag{27}$$

Since the bare dual Green's function calculated in the independent QMC run for the reference system, it is fully translationally invariant $\tilde{G}^0_{34} \equiv \tilde{G}^0(3-4)$ and we used Fourier transform to calculate the K-space dual Green's function $\tilde{G}^0_k$.

In the K-space the subtractions of disconnected part has the following form

$$\tilde{g}^s_{kk'} = g^s_{kk'} - g_k \delta_{kk'} \tag{28}$$

For transformation of the vertex γ^d_{1234} in Eq. (9)within the QMC step in the K-space we take into account that indices $3, 4$ are "diagonal" in k-spcae due to multiplication

by translationally invariant dual Green's function $\tilde{G}^0_{34}$ which transforms as $\tilde{G}^0_k \delta_{kk'}$ and indices $1, 2$ become translationally invariant after QMC-summation, which finally leads us to the following equation for final spin-up components of the first order dual self-energy $\tilde{\Sigma}_k$ in the spinor-form with normalization $Z = (\beta N)^2 Z_{QMC}$

$$\tilde{\Sigma}^{\uparrow\uparrow}_k = \frac{-1}{Z} \sum_{QMC} \sum_{k'} \left[\left(\tilde{g}^{\uparrow}_{kk} \tilde{g}^{\uparrow}_{k'k'} - \tilde{g}^{\uparrow}_{kk'} \tilde{g}^{\uparrow}_{k'k} \right) \tilde{G}^{\uparrow\uparrow}_{k'} + \tilde{g}^{\uparrow}_{kk} \tilde{g}^{\downarrow}_{k'k'} \tilde{G}^{\downarrow\downarrow}_{k'} \right] \tag{29}$$

$$\tilde{\Sigma}^{\downarrow\downarrow}_k = \frac{-1}{Z} \sum_{QMC} \sum_{k'} \left[\left(\tilde{g}^{\downarrow}_{kk} \tilde{g}^{\downarrow}_{k'k'} - \tilde{g}^{\downarrow}_{kk'} \tilde{g}^{\downarrow}_{k'k} \right) \tilde{G}^{\downarrow\downarrow}_{k'} + \tilde{g}^{\downarrow}_{kk} \tilde{g}^{\uparrow}_{k'k'} \tilde{G}^{\uparrow\uparrow}_{k'} \right] \tag{30}$$

$$\tilde{\Sigma}^{\uparrow\downarrow}_k = \frac{+1}{Z} \sum_{QMC} \sum_{k'} \tilde{g}^{\uparrow}_{kk'} \tilde{g}^{\downarrow}_{k'k} \tilde{G}^{\uparrow\downarrow}_{k'} \tag{31}$$

Note, that for AFM-field we need to substitute:

$$\tilde{g}^{\downarrow}_{kk'} \Rightarrow \tilde{g}^{\uparrow}_{(k+Q),(k'+Q)} \tag{32}$$

Correspondently, for SC-Dw field we need to substitute:

$$\tilde{g}^{\downarrow}_{kk'} \Rightarrow -\tilde{g}^{\uparrow}_{-k',-k} \tag{33}$$

Additional normalisation factor $\frac{1}{(\beta N)^2}$ comes from the Fourier transform in k and from the $\mathbf{k}'$-sum with N-lattice cites and summation over Matsubara frequency: $\frac{1}{\beta} \sum_{\nu'}(...)$. For paramagnetic calculations we average over two spin projections.

Corresponding lattice matrix Green's function reads:

$$G_k = \left[\left(g_k + \tilde{\Sigma}_k \right)^{-1} - \tilde{t}_k \right]^{-1} \tag{34}$$

In the case of AFM-field we have final Green's function for paramagnetic reference system

$$G_k = \left[\begin{pmatrix} g_k + \tilde{\Sigma}^{\uparrow\uparrow}_k & \tilde{\Sigma}^{\uparrow\downarrow}_k \\ \tilde{\Sigma}^{\downarrow\uparrow}_k & g_{k+Q} + \tilde{\Sigma}^{\downarrow\downarrow}_k \end{pmatrix}^{-1} - \begin{pmatrix} \tilde{t}_k & 0 \\ 0 & \tilde{t}_{k+Q} \end{pmatrix} \right]^{-1} \tag{35}$$

with $\tilde{\Sigma}^{\downarrow\uparrow}_k = \left(\tilde{\Sigma}^{\uparrow\downarrow}_k \right)^*$. Final magnetic moment can be calculated via

$$m = \sum_{k'} Tr(\sigma_x G_k) \tag{36}$$

which include Matsubara sum with factor β

For the HTSC-field corresponding Green's function reads

$$G_k = \left[\begin{pmatrix} g_k + \tilde{\Sigma}^{\uparrow\uparrow}_k & \tilde{\Sigma}^{\uparrow\downarrow}_k \\ \tilde{\Sigma}^{\downarrow\uparrow}_k & -g^*_k + \tilde{\Sigma}^{\downarrow\downarrow}_k \end{pmatrix}^{-1} - \begin{pmatrix} \tilde{t}_k & 0 \\ 0 & -\tilde{t}^*_k \end{pmatrix} \right]^{-1} \tag{37}$$

with final superconducting order parameter

$$\Delta = \sum_{k} Tr(\sigma_x G_k)(\cos k_x - \cos k_y) \tag{38}$$

1 Final Expressions

We separate Hartree (direct, H-constant) and Fock (exchange, F-k-dependent) contribution to $\tilde{\Sigma}^{(1)}$ and average over spins gives the factor $\frac{1}{2}$ in paramagnetic state, since $\tilde{G}_k$ is spin-independent.

Fist order DF-QMC correction:

$$\tilde{\Sigma}_k^{(1)} = -\frac{1}{2} \sum_{QMC} \left[\left(\tilde{g}_{kk}^{\uparrow} + \tilde{g}_{kk}^{\downarrow} \right) H_c - F_k \right] \tag{39}$$

where

$$H_c = \sum_{k'} \left(\tilde{g}_{k'k'}^{\uparrow} + \tilde{g}_{k'k'}^{\downarrow} \right) \tilde{G}_{k'} \tag{40}$$

and

$$F_k = \sum_{k'} \left(\tilde{g}_{kk'}^{\uparrow} \tilde{g}_{k'k}^{\uparrow} + \tilde{g}_{kk'}^{\downarrow} \tilde{g}_{k'k}^{\downarrow} \right) \tilde{G}_{k'} \tag{41}$$

DATA AVAILABILITY The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Competing Interests The authors declare no competing interests.

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