Dual fermion approach to the two-dimensional Hubbard model: Antiferromagnetic fluctuations and Fermi arcs

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We present an efficient diagrammatic method to describe nonlocal correlation effects in lattice fermion Hubbard-like models, which is based on a change of variables in the Grassmann path integrals. The new fermions are dual to the original ones and correspond to weakly interacting quasiparticles in the case of strong local correlations in the Hubbard model. The method starts with dynamical mean-field theory as a zeroth-order approximation and includes non-local effects in a perturbative way. In contrast to cluster approaches, this method utilizes an exact transition to a dual set of variables. It therefore becomes possible to treat vertices of an effective single-impurity problem as small parameters. This provides a very efficient interpolation between band-like weak-coupling and atomic limits. The method is illustrated on the two-dimensional Hubbard model. The antiferromagnetic pseudogap, Fermi-arc formations, and non-Fermi-liquid effects due to the van Hove singularity are correctly reproduced by the lowest-order diagrams. Extremum properties of the dual fermion approach are discussed in terms of the Feynman variational principle.

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I. INTRODUCTION

One of the most successful theories of strongly correlated fermions on a lattice is dynamical mean-field theory (DMFT)\(^1\). Physically, this approach treats the local spin and orbital fluctuations of the correlated electrons in a correct self-consistent way, while the spatial intersite correlations on the lattice are neglected. The non-perturbative DMFT approach is successful, because a number of the most important correlation effects are indeed related to local fluctuations. For example, DMFT describes correctly such phenomena as the local moment formation in itinerant magnets\(^2\), some aspects of Kondo physics\(^3\), and the Mott insulator-to-metal transition on a lattice with a large connectivity in high-dimensional materials\(^4\).

On the other hand, there is increasing evidence that the non-locality of spatial correlations plays an important role, particularly for the Luttinger liquid physics of low-dimensional correlated systems\(^5\), d-wave pairing in quasi two-dimensional cuprates\(^6,5\), and non Fermi-liquid behavior due to van-Hove singularities in two-dimensional systems\(^7,8,9\). Moreover, angle-resolved photoemission spectra of three-dimensional ferromagnetic iron shows appreciable k-dependent self-energy effects\(^10\).

The most obvious generalizations of DMFT that takes into account the short-range non-local fluctuations are the so-called cluster DMFT approximations, in real or k-space\(^11,12\). In these methods, correlations are assumed to be localized within a cluster including several lattice sites. Cluster methods do catch the basic physics of d-wave pairing and anti-ferromagnetism in high-T\(_c\) superconductors\(^13,14\) and the effects of inter-site Coulomb interaction in transition-metal oxides\(^15\). At the same time, the complicated k-dependence of the self-energy close to the Fermi surface, giving rise to Luttinger liquid formation is related to long-range fluctuations and therefore cannot be described within cluster approaches. For the same reason, cluster methods hardly can handle the effects due to van Hove singularities or nesting\(^7,9\). Another drawback of the cluster methods is that the specific choice of the cluster and corresponding self-consistency condition is not unique. Different self-consistency conditions (e.g. DCA\(^12\) and free-cluster CDMFT\(^11\)) or periodization schemes (e.g. self-energy and cumulant periodization\(^14\)) can result in physically different solutions. For example, the critical temperature of the d-wave superconducting transition of the doped Hubbard model is different in DCA calculations\(^12\) and for then 2 x 2 free cluster\(^14\).

The present paper is devoted to an alternative extension of DMFT, which operates with a single-site impurity problem and treats spatial nonlocality in a diagrammatic way.

Let us first recall the key DMFT equations. Formally, the assumption of local correlations means that the environment of a correlated atom can be replaced with a Gaussian effective medium. Consequently, the lattice problem reduces to the impurity problem. The later is described by the effective impurity action

\[ S_{\text{imp}} = S_{\text{at}} + \sum_{\omega,\sigma} \Delta_{\omega,\sigma} c_{\omega,\sigma}^\dagger c_{\omega,\sigma}, \]  

where \(S_{\text{at}}\) is an action of the isolated or bare atom, and the second term is the hybridization due to the rest of the lattice. An important property of the DMFT approach is that this hybridization function has non-trivial frequency dependence, so that the approximation catches the physics of local fluctuations of spin, charge, and orbital degrees of freedom. For example, it is vital, for the
description of Kondo physics\(^3\).

It is obvious that the impurity problem is much simpler than the original lattice one. Nowadays, a number of numerically efficient impurity solvers are available. In particular, these solvers allow one to calculate the Green's function of the impurity problem \(g_{\omega,\sigma}\) on the Matsubara frequencies axis. This is the only property of the impurity problem entering in the DMFT self-consistent equations. The DMFT approximation for the Green's function of the initial lattice problem corresponds to the following expression

\[
G_{\omega k\sigma}^{\text{DMFT}} = \frac{1}{g_{\omega,\sigma}^{-1} + \Delta_{\omega,\sigma} - \epsilon_k}.
\]  

(2)

One can see from this equation that the self-energy is local in DMFT, since the momentum dependence of \(\epsilon_k\) is not renormalized. The hybridization function \(\Delta\) satisfies the self-consistency condition of DMFT,

\[
G_{\omega k\sigma}^{\text{DMFT}} = g_{\omega,\sigma},
\]  

(3)

where \(G_{\omega k=0} = N^{-1} \sum_k G_k\) is the local part of the Green's function \(2\) of the lattice with \(N\) sites.

In order to understand the main idea of the present work, let us first describe in a simple way the DMFT condition \(3\). If we consider the case of a truly Gaussian system then the DMFT approach becomes exact. For this case, equation \(3\) is trivial. Indeed, to obtain the impurity problem for the site \(j\), one integrates out truly Gaussian degrees of freedom for other sites. This exact procedure does not change the properties of the electron motion at the site \(j\), so the local part of the Green's function before integration must equal the Green's function after the integration, \(G_{\omega k=0} = g\). Turning back to the general case of a non-Gaussian ensemble, we note that among different properties of the impurity model, the DMFT scheme uses only the local Green's function \(g_{\omega,\sigma}\). Once \(g_{\omega,\sigma}\) is known, the approximation does not differ between Gaussian and non-Gaussian cases. Therefore, if a certain equation for \(g_{\omega,\sigma}\) is established for the Gaussian limit, it must also remain valid for the general case.

As it follows from the previous discussion, the DMFT equations are essentially the formulae for the Gaussian limit, renormalized in terms of the Green's function of the impurity problem. It turns out that the resulting theory works well, not only in the case of weakly interacting systems, but also in the atomic limit case, which is very different from a Gaussian system. A good interpolation between the two different limits is a key advantage of the DMFT approach.

Starting with the above interpretation of DMFT, it is natural to discuss a possible extension of this theory. Such an extension should be based on the perturbation series near the Gaussian limit, renormalized in terms of the impurity problem. The lowest-order term of such a theory should restore the DMFT result, whereas higher-order corrections would describe spatial non-locality. A properly constructed theory of this kind would describe both short- and long-range fluctuations and will not suffer from the periodization problems of cluster DMFT.

Unfortunately, the straightforward construction of such an extension meets serious difficulties. The problem is that the extension is not unique. Beyond DMFT, there are many ways to choose the renormalization procedure, to define the hybridization function for the impurity problem and other quantities. One can formulate the major requirements for the desirable non-local correlated theory, they include:

- at least in the Gaussian and atomic limits, the theory should become a regular series around DMFT, with an explicit small parameter;
- the basic conservation laws should be fulfilled in the theory;
- the choice of hybridization function should be optimal, in a certain sense;
- there should be good practical convergence of the series: the leading corrections should capture most of the non-local physics;
- last but not least, the equations of the theory must be easy enough for practical calculations.

There have been several previous attempts to construct a proper theory of this kind\(^{16,17,18}\). These approaches require a solution of ladder-like integral equations for the complete vertex \(\Gamma\) and the subsequent use of the Bethe-Salpeter equation to obtain the Green's functions. The first step exploits the vertex part of the effective impurity problem, whereas the second step uses just the bare interaction parameter \(U\). We do not know of detailed tests of these approaches\(^{16,17,18}\), but we suspect that the presence of bare \(U\) in the theory makes it suitable for the metallic phases only. We also note that ladder-like integral equations are hard for practical calculations.

In this paper, we describe in detail a formalism fulfilling all the criteria from the above list. A preliminary version of this method was published in Ref.\(^{19}\). The method is based on the transition to the new set of variables, called the dual ensemble. The procedure utilizes a Hubbard-Stratonovich transformation for the Gaussian part of the action. Several years ago, this trick was first proposed for classical fluctuation fields\(^{20}\). For a strong coupling expansion of the Hubbard model around the atomic limit without hybridisation function, the equivalent Hubbard-Stratonovich transformation has been proposed in different papers\(^{21,22}\). A similar procedure for fermions with general non-local interactions have been discussed recently\(^{23}\). Also we would like to mention a much earlier work\(^{24}\) for classical fields. Although, it used a different formalism\(^{24}\), the resulting diagram series resembles ours.

The paper is organized as follows. Section II is devoted to the general theoretical framework. Section III describes the application of the non-local theory to the
problem of the antiferromagnetic pseudogap and the formation of Fermi arcs in the two-dimensional Hubbard model for high-temperature superconducting cuprates. In the Appendix A we discuss how the many-particle excitations for the initial and dual system are related. In the Appendix B the functional minimization derivation of the self-consistent DMFT condition is discussed.

II. DUAL FERMION FORMALISM: BEYOND DMFT

A. Definitions

We start from the two-dimensional Hubbard model with the corresponding imaginary-time action

\[ S[c, c^*] = \sum_{w, k, \sigma} (\epsilon_k - \mu - i\omega) c^\dagger_{w, k, \sigma} c_{w, k, \sigma} + U \sum_i \int_0^\beta n_{i+1, i, \sigma} d\tau. \] (4)

Here \( \beta \) and \( \mu \) are the inverse temperature and chemical potential, respectively, \( \omega = (2j+1)\pi/\beta, j = 0, \pm 1, \ldots \) are the Matsubara frequencies, \( \tau \) is imaginary time, \( \sigma = \uparrow, \downarrow \) is the spin projection. The bare dispersion law is \( \epsilon_k = -2t(\cos k_x + \cos k_y) \), \( c^\dagger, c \) are Grassmann variables, \( n_{i, \sigma} = c^\dagger_{i, \sigma} c_{i, \sigma} \), where the indices \( i \) and \( k \) label sites and quasi-momenta.

In the spirit of the DMFT, we introduce a single-site reference system (an effective impurity model) with the action

\[ S_{\text{imp}} = \sum_{\omega, \sigma} (\Delta_\omega - \mu - i\omega) c^\dagger_{\omega, \sigma} c_{\omega, \sigma} + U \int_0^\beta n_{i+1, i, \sigma} d\tau, \] (5)

where \( \Delta_\omega \) is a yet undefined hybridization function describing the interaction of the effective impurity with a bath. We assume that all properties of the impurity problem such as single-particle Green's function \( g_\omega \), and higher momenta can be calculated. In particular, we will use the fourth-order vertex \( \gamma^{(4)}_{1234} = g_{11'}^{-1} g_{22'}^{-1} (\chi_{12}^\dagger \chi_{34}^\dagger - g_{13'} g_{24'}) g_{33'} g_{44'} \) (here, \( \chi \) is a two-particle Green's function of the impurity problem, and indices stand for a combination of \( \sigma \) and \( \omega \), for example \( g_{11'} \) means \( g_{\sigma_1 \omega_1, \sigma_1' \omega_1'} \)).

Our goal is to express the Green's function \( G_{\omega, k} \) and other properties of the lattice problem of Eq. (4) via the quantities for the impurity problem.

B. Dual variables: exact formulas

Since \( \Delta \) is independent of \( k \), the lattice action (4) can be represented in the following form

\[ S[c, c^*, f, f^*] = \sum_i S_{\text{imp}}[c_i, c^*_i] - \sum_{\omega, k, \sigma} (\Delta_\omega - \epsilon_k) c^\dagger_{\omega, k, \sigma} c_{\omega, k, \sigma}. \] (6)

We utilize a dual transformation to a set of new Grassmann variables \( f, f^* \). The following identity

\[ e^{A^2} c_{\omega, k, \sigma} c_{\omega, k, \sigma} = \left( \frac{A}{\alpha} \right)^2 \int e^{-\alpha (c_{\omega, k, \sigma} f^*_{\omega, k, \sigma} + f_{\omega, k, \sigma} c_{\omega, k, \sigma}) - A^2 f^*_{\omega, k, \sigma} f_{\omega, k, \sigma} df^*_{\omega, k, \sigma} df_{\omega, k, \sigma}, \] (7)

is valid for arbitrary complex numbers \( A \) and \( \alpha \). We chose \( A^2 = (\Delta_\omega - \epsilon_k) \) for each set of indices \( \omega, k, \sigma \). The quantity \( \alpha \) remains yet unspecified, but we require it to be dispersionless; \( \alpha = \alpha_{\omega, \sigma} \).

With this identity, the partition function of the lattice problem \( Z = \int e^{-S[c, c^*, f, f^*]} Dc^* Dc \) can be presented in the form \( Z = \int e^{-S[c, c^*, f, f^*]} Df^* Df Dc^* Dc \), where

\[ S[c, c^*, f, f^*] = -\sum_{\omega, k} \ln \left( \alpha_{\omega, \sigma}^2 (\Delta_\omega - \epsilon_k) \right) + \sum_i S_{\text{imp}}[c_i, c^*_i] + \sum_{\omega, k, \sigma} \left[ \alpha_{\omega, \sigma} (f^*_{\omega, k, \sigma} c_{\omega, k, \sigma} + c^*_{\omega, k, \sigma} f_{\omega, k, \sigma}) + \alpha_{\omega, \sigma}^2 (\Delta_\omega - \epsilon_k)^{-1} f^*_{\omega, k, \sigma} f_{\omega, k, \sigma} \right]. \] (8)

As a next step, we establish an exact relation between the Green's function of the initial system \( G_{\tau, \tau', i, i'} = -< Tc_{\tau, i} c^*_{\tau', i'} > \) and that of the dual system \( G_{\tau, \tau', i, i'}^{\text{dual}} = -< Tf_{\tau, i} f^*_{\tau', i'} > \). To this aim, we can replace \( \epsilon_k \rightarrow \epsilon_k + \delta \epsilon_{\omega, k} \) with a differentiation of the partition function with respect to \( \delta \epsilon_{\omega, k} \). Since we have two expressions for the action (4) and (8), one obtains

\[ G_{\omega, k} = (\Delta_\omega - \epsilon_k)^{-1} \alpha_{\omega, \sigma} G_{\omega, k}^{\text{dual}} \alpha_{\omega, \sigma} (\Delta_\omega - \epsilon_k)^{-1} + (\Delta_\omega - \epsilon_k)^{-1}. \] (9)

Similar relations hold also for higher-order momenta, as Appendix A describes.

The crucial point is that the integration over the initial variables \( c^*_i, c_i \) can be performed separately for each lattice site, since \( \alpha \) is local and \( \sum_k (f^*_k c_k + c^*_k f_k) = \sum_i (f^*_i c_i + c^*_i f_i) \). For a given site \( i \), one should integrate out \( c^*_i, c_i \) from the action that equals

\[ S_{\text{site}}[c_i, c^*_i, f_i, f^*_i] = S_{\text{imp}}[c_i, c^*_i] + \sum_{\omega} \alpha_{\omega, \sigma} (f^*_{\omega} c_{\omega} + c^*_{\omega} f_{\omega}). \] (10)
We finally obtain an action $S$ depending on the new variables $f, f^\ast$ only:

$$
S[f, f^\ast] = -\sum_{\omega_k} \ln \left(\alpha_{\omega, \sigma}^2 (\Delta_\omega - \epsilon_k)\right) - \sum_{\omega_k} \ln z_i^{imp} + \sum_{\omega_k} \alpha_{\omega, \sigma} \left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega\right) \alpha_{\omega, \sigma} f_{\omega, k^\sigma}^* f_{\omega, k^\sigma} + \sum_i V_i,
$$

where $z_i^{imp} = \int e^{-S_{imp}} [c_i^\dagger, c_i] Dc_i^\dagger Dc_i$, and the dual potential $V_i \equiv V[f_i, f_i^\ast]$ is defined from the expression

$$
\int e^{-S_{dual}} [c_i^\dagger, c_i, f_i^\ast, f_i] Dc_i^\dagger Dc_i = z_i^{imp} \epsilon \sum_{\omega_k} \alpha_{\omega, \sigma}^2 g_\omega f_{\omega, k^\sigma}^* f_{\omega, k^\sigma} - V[f_i, f_i^\ast].
$$

The Taylor series for $V[f_i, f_i^\ast]$ can be obtained from the expansion of this definition in powers of $f_i, f_i^\ast$. One can see that (11) defines $V$ in such a way that this series starts from the quartic term, $\propto f^4 f^4$. Later on we take, for convenience:

$$
\alpha_{\omega, \sigma} = g_\omega^{-1},
$$

as it gives a particularly simple form of $V$. In this case the leading term in $V$ is $-\frac{1}{4} \gamma^{(3)} (f_i f_i^\ast)^2 f_i f_i^\ast$. Further Taylor series terms yield similar combinations including $\gamma^{(n)}$ of higher orders.

Thus we see that in the dual action, the interaction terms remain localized in space, but are they non-local in imaginary time, since, for example, $\gamma^{(3)}$ depends on the three independent Matsubara frequencies. Except for this point, the action (11) formally resembles (4).

There is a point which is worthwhile to discuss here: one can formally apply the transformation (7) with some new hybridization function to the dual system (11), and thus obtain a sequence of changes to new variables. It is useless, however, since mathematically, these transformations form a group. It is easy to show that any sequence of the transformations (7) corresponds to a single change of variables with a certain $\Delta$. Moreover, there is an inverse change of variables, that allows to obtain $S[c, c^\ast]$ back from the $S[f, f^\ast]$. It is given just by Eq.(7) with $A$ replaced with $\alpha A^{-1}$.

### C. Gaussian approximation for dual ensemble and the relation to DMFT

Since the transformation from the initial system (4) to the action (11) contains no approximations, it is equally hard to describe exactly the properties of $c_i^\dagger, c_i$ fermions as thereof $f_i^\ast, f_i$ dual-fermions. The main idea of switching to the new variables is that, for a properly chosen $\Delta$, correlation properties of the $f_i^\ast, f_i$ system are simpler than for the $c_i^\dagger, c_i$ original model. In other words, the magnitude of the nonlinear part in the dual action can be effectively decreased by the proper choice of $\Delta$. To illustrate this statement, let us just neglect $V$ in (11). We denote the Green’s function for such Gaussian approximation for the dual potential with calligraphic letters. The expression (11) corresponds to

$$
G^\text{dual}_{\omega, k} = -g_\omega \left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega\right)^{-1} g_\omega.
$$

Being combined with the identity (9), this gives the formula

$$
G_{\omega, k} = (g_\omega^{-1} + \Delta_\omega - \epsilon_k)^{-1}.
$$

One can recognize that this is exactly a DMFT expression for the Green’s function. Therefore we conclude that for a properly chosen $\Delta$ already a Gaussian approximation for the dual potential yields a reasonable result, as DMFT does. It is important to point out that DMFT works well for the whole range of the parameters. In contrast, the Gaussian approximation for the atomic limit of the initial model (4) makes no sense. In that aspect, the dual potential $V$ is indeed smaller than $U$.

An argumentation can be presented to justify that the DMFT value of $\Delta$ is a proper choice for the Gaussian approximation (14, 15). One of the reasons is described in the Appendix B. It turns out that Feynman minimization criterion for the Gaussian trial action, been formulated for the dual ensemble, gives exactly the DMFT hybridization function. Another argument is presented in the following subsection.

Once the dual potential is taken into account, it yields a correction to the DMFT result. It is useful to introduce the dual self-energy

$$
\Sigma^\text{dual} \equiv G^{-1} - G^{-1}_\text{dual},
$$

and the correction to the DMFT self-energy

$$
\Sigma' \equiv G^{-1} - G^{-1}.
$$

With these quantities, we can reexpress the exact relation (9) in a particularly simple form

$$
\Sigma_{\omega, k}^{-1} = g_\omega + \left(G_{\omega, k}^{-1}\right)^{-1}.
$$

We note that this expression relates quite different quantities: $\Sigma^\text{dual}$ and $\Sigma'$ characterize the corresponding lattice problems and carry, in general, both momentum- and frequency-dependence, whereas $g$ comes from the impurity model and is local in space.

### D. Diagram series: general properties and the choice of hybridization function

The main idea of our method is to consider a diagrammatic expansion with respect to the dual potential $V$. 
We will later demonstrate that already low-order diagrams of such a series bring an important information about non-local correlations. The basic reasoning for this is presented in the previous subsection: since the value of \( V \) is in certain sense small, the first few terms of the perturbation series with respect to \( V \) can make sense. More detailed discussion about the small parameters of the theory are presented in the next sections; let us first present the general properties of the diagrams under consideration.

The rules of diagram construction are quite similar to the usual Matsubara diagram technique. The only difference from the standard perturbation scheme is that the interaction operator \( V \) is not purely of the 4-th order form \( f^*f^*f^*f \), and therefore vertices in the diagrams are not necessarily four-leg, but may formally have any even number of legs. For the choice (13), these vertices are essentially \( \gamma(n) \). They are connected with the lines being the dual Green’s functions. Some of the diagrams contributing to the dual self-energy are presented in Figure (1).

We use the skeleton diagrams with renormalized Green’s functions, so that the lines are complete \( G_{\text{dual}} \), and not \( G_{\text{dual}} \). The reason to use the skeleton-diagram expansion for the dual self-energy is that it makes possible to obtain conserving theories, similarly to conventional diagram technique\[25\]. The Baym criterion of a conservative theory is the existence of a functional of the Green function \( \Phi[G] \) such that \( \frac{\partial \Phi}{\partial G} = \Sigma \). Once this functional is described by certain skeleton diagrams, taking the derivative means just cutting the lines in that diagram. For example, the diagrams (a) and (b) for the self-energy come from diagrams (a\(_b\)) and (b\(_b\)), shown in Figure(2) (of course, care should be taken of the numerical factors). Second-order differentiation with respect to \( G \) gives the two-particle quantities. Such a procedure automatically produces a theory fulfilling the conservation laws for energy, momentum, particle numbers etc.

In our consideration, the usage of skeleton diagrams describes a corresponding Baym functional \( \Phi_{\text{dual}}[G_{\text{dual}}] \) with the functional derivative being \( \Sigma_{\text{dual}} \). Therefore, it produces a conservative approximation for the dual ensemble. Then it turns out that the exact transformations (9) and (A5) give a conserving description of the initial system. Simply, the conservation laws imply certain selection rules for \( G \) and \( \Gamma \), and (9, A5) clearly preserve those selection rules during the transformation from dual to initial quantities. More precisely, the conserving character of an approximation in fact means that there exists some conserving dual action \( S[f, f^*] \), exactly corresponding to this approximation. Since there is a one to one correspondence between \( S[f, f^*] \) and \( S[c, c^*] \) (see the end of Section II B), we conclude that the initial system described by a certain \( S[c, c^*] \) is also conserving.

Until now, the hybridization function \( \Delta \) was formally not specified. Now, we establish a condition for \( \Delta \) that corresponds to a particular condition for the diagrammatic series. Let us again consider the DMFT. Suppose that we want to obtain the DMFT result without DMFT loops, that is using \( \Delta_{\text{DMFT}} \), not fulfilling (B5). Formally, it is possible: one should just sum up all the diagrams containing a single vertex (diagrams a, a’, a” etc.). Since these diagrams give exactly the DMFT self-energy, such a procedure would indeed recover the DMFT result for an arbitrary hybridization function. The special DMFT choice of \( \Delta \) just allows to eliminate such an infinite summation, since (B6) eliminates all the diagrams containing a simple closed loop. It is reasonable to keep this property in higher approximations, that is to require

\[
G_{\omega, \tau, r = 0}^{\text{dual}} = 0
\]  

(19)

as a condition for \( \Delta \). Then, all the diagrams with simple closed loops drop out from the calculation. Note that these diagrams however should be taken into account while taking the functional derivatives. For example, the DMFT vertex part \( \Gamma_{\text{dual}} = \gamma^{(4)} \) comes out from the differentiation of diagram (a). Finally, the condition (19) obviously passes into (B6) at the DMFT limit. Therefore, until the corrections to DMFT are significant, one can approximate \( \Delta_{\text{DMFT}} \) with the DMFT hybridization function.

The vanishing of the closed loops seriously reduces the number of the low-order dual diagrams. In most of the practical calculations presented below we consider a single diagram (b). It is clear that any reasonable expansion starts from this perturbation, and that this diagram already incorporates some non-local physics. The corresponding formula for the dual self-energy reads (spin and orbital indices are omitted):

\[
\Sigma_{\omega, r}^{\text{dual}} = \frac{1}{2\beta^2} \sum_{\omega + \omega' = \omega_0 + \omega_1} \gamma^{(4)}_{\omega_0, \omega_1, \omega_2, \omega_3, \omega_4, \omega_5} \gamma^{(4)}_{\omega_5, \omega_4, \omega_3, \omega_2, \omega_1, \omega_0} C_{\omega, r}^{\text{dual}} C_{\omega', r}^{\text{dual}} C_{\omega', r}^{\text{dual}}
\]

(20)
E. Causal properties

Beyond conservation laws, the Green's function should be causal. The retarded Green's function $G^R(t)$, that is an analytical continuation of $G$ to the real-time axis, should vanish for negative time:

$$G^R(t < 0) = 0. \quad (21)$$

In the Fourier representation, condition (21) implies the analyticity of $G_\omega$ in the upper complex plane, as this follows directly from the definition of the Fourier transform. The inverse is also true. If the Fourier transform of a function is analytical in the upper-plane, the function is causal. To prove this statement, it is enough to transform the integration contour of the inverse Fourier transform away from the real axis.

Frequently, the causality principle is associated with the positiveness of the imaginary part of the Green's function in the real-frequency domain. For dual Green's function, this can lead to certain misunderstanding. It is clear from condition (19) that the imaginary part of $G^{dual}$ cannot be always-positive. However, this issue is purely formal. Condition (21) itself does not imply that $\text{Im}G_\omega$ is positive. A trivial counter-example is the function $-G^R$. It fulfills (21), and has an always-negative imaginary part. We will argue the same for $G^{dual}$. It fulfills (21). Although, its imaginary part is not always-positive.

Let us illustrate this statement at the zeroth order of the theory, single-site DMFT. It has been proven that the causality of $G$ and $g$ is preserved even if the Green’s function is causal, so $G$ and $g$ fulfill (21). One can easily check, from the expressions (14, 15), for the case of DMFT, a simple relationship holds: $G^{dual} = G - g$. It is immediately clear from this formula, since $G$ and $g$ are causal, $G^{dual}$ also fulfills (21). Note again, both condition (19) is fulfilled in DMFT, and $-\text{Im}G^{dual}$ is therefore essentially non-positive.

Let us now consider the dual-fermion theory beyond DMFT. We will show that, if the hybridization function $\Delta$ is causal, the resulting Green’s function $G$ is also causal. First of all, the causality of $\Delta$ is inherited from $G$ and $g$ (14, 15). Therefore, the dual system is characterized by the casual bare propagator $G^{dual} = G - g$ and casual interaction operator. Therefore, the theory with skeleton diagrams results in a causal $G^{dual}$. Finally, it should just be proven that the causality $G^{dual}$ means the causality of $G$. The later statement follows from the exact relation (9). Indeed, since $\alpha \equiv g_\omega$ does not have zeros in the upper-plane, $g^{-1}$ is analytical. The same is true for the quantity $(\Delta - \epsilon)^{-1}$. Therefore, the entire right-hand side of (9) is analytical in the upper-plane. This implies the causality of $G$.

In the calculation procedure described below, we always start from a causal $\Delta$ and change it iteratively to deliver condition (19). We will argue that such an iteration procedure preserve the causality of $\Delta$. Therefore, the entire theory is causal.

Finally, let us recall the issue of the positiveness of $-\text{Im}G$ in the complex upper-plane. Actually, this is related with the positiveness of the residuals, as it follows from the Lehmann representation $G = \sum \frac{Z_{im}}{\omega - \omega_{mn} + i \delta_{mn}}$.

Here, the causality follows from the positiveness of $\delta$, whereas the requirement $Z > 0$ ensures that $-\text{Im}G > 0$. For our theory, we were not able to prove the positivity of the residuals formally. However, we do not consider this as a serious drawback, since our practical calculations always produce undoubtly positive residuals.

F. Small parameter in the extreme cases

An important property of the DMFT approach is that it becomes exact for the two opposite cases of a non-interacting Gaussian system and of an extreme strong-coupling limit corresponding to the atomic limit\(^1\). The dual-fermion formalism inherits this property; moreover the corresponding smallness appears in the diagrams in a simple form. Let us first consider the strong-coupling limit $\epsilon \to 0$. It is useful to estimate the DMFT dual Green’s function $G$, defined by the formula (14) and the condition (19). For a pure atomic limit $\epsilon \to 0$, the Green’s function is local, $g_{\alpha \neq 0} = 0$. However, the local part of the Green’s function also vanishes due to the condition (19). Formally, $G \to 0$ as $\Delta \to 0$. The smallness of $\epsilon$ and $\Delta$ allows the approximate estimation of the dual Green’s function near the atomic limit. It gives $G_{\alpha \beta} \approx g_{\alpha \beta} \epsilon g_{\alpha \beta}$. Since the DMFT is almost exact near the atomic limit, the same estimation is valid for $G^{dual}$. Consequently, near the atomic limit the lines in the dual diagrams carry a small factor $g_{\alpha \beta}$.

On the other hand, for the opposite weak-coupling limit $U \to 0$, the vertex parts of the impurity problem can be estimated as $\gamma \propto U$, $\gamma \propto U$, etc. Therefore, for the weak-coupling limit the vertices in the dual diagrams are manifestly small.

The presence of a small parameter in these two limits does not guaranty a good interpolation between them. It should however be mentioned, that the scheme performs well if the corrections to DMFT are small: for this case we deal in fact with a perturbation series around DMFT. The validity of the method for more general situations should be checked in practical calculation. This practical validity depends on the particular choice of diagrammatic approximation for $\Sigma^{dual}$. In this context, it is worth to discuss the choice of hybridization function $\Delta$.

G. Calculation procedure

In practical calculations the solution was obtained iteratively, similarly to the DMFT loop. The iterative scheme is presented in Figure 3. It includes the big (outer) and small (inner) loops. The small loop is devoted to obtain the dual Green’s function and self-energy, given the solution of the impurity model with certain...
III. APPLICATION TO THE HUBBARD MODEL

In the next sections, we present the results of our calculations for the 2D Hubbard model. We start with the half-filled case with nearest-neighbor hopping $t' = 0$ lattice. We compare our data with direct QMC simulations on a finite Hubbard lattice, which are relatively simple due to the absence of the sign problem for the half-filled Hubbard model.

Properties of the half-filled Hubbard model are well-known and are mostly related to the antiferromagnetic phenomenon and Mott metal-insulator transition. Local magnetic moment on atoms are formed and tend to ordered into an antiferromagnetic lattice due to the effective super-exchange coupling. At zero temperature, the antiferromagnetism arises already at $U = 0^+$, because of the perfect nesting. At finite temperature, the true antiferromagnetism is destroyed by the long-range fluctuations. However, short-range antiferromagnetic correlations are still present. Short-range antiferromagnetic ordering manifests itself as the strong pseudogap in the local electron spectral function.

We consider the system with $t = 0.25$ at inverse temperature $\beta = 20$, with different values of $U$. Since the temperature is relatively high, it is enough to use the reference data obtained just for the $8 \times 8$ lattice QMC simulation, with subsequent maximum-entropy continuation of the data to obtain local density of states (DOS). The result for paramagnetic calculation is presented in Figs. 4, 6 (thin solid line). These results show that the narrow antiferromagnetic pseudogap is formed at approximately $U = 1.0$. For larger $U$, the DOS contains also a wider Mott gap, having a halfwidth of about $U/2$. At $U = 2.0$, the system shows essentially Mott-insulator DOS; the effect of antiferromagnetism in this case consists in the sharp shoulders of the Mott gap.

To understand better the physics of the half-filled Hubbard model, it is worth to analyse the behavior of the electronic self-energy $\Sigma$. At small $U$, this is a small regular correction to the dispersion law $\epsilon_k$. It follows from the weak-coupling analysis that $\text{Im} \Sigma$ is strongly anisotropic in this regime, with peaks near $[0, \pm \pi], [\pm \pi, 0]$ points. In contrast, for the truly antiferromagnetic gap, $\Sigma_k$ would have a pole at the Fermi surface. The residue of this pole is the same at all points of the Fermi surface. For large enough $U$ this pole is somehow shifted from the real-frequency axis due to long-range thermal fluctuations, but the qualitative picture remains the same: a sharp peak in $\text{Im} \Sigma$, with almost constant magnitude along the Fermi surface.

It is well-known that doping changes the physics of the Hubbard model substantially. First of all, already a few-percent doping suppresses the antiferromagnetism. At higher doping values there is a trend to $d$-wave superconductivity. A superconducting phase has been obtained in various cluster-DMFT calculations13,28 near the optimal doping of about 15%. This agrees well with the phase...
diagram of high-$T_c$ cuprates. The pseudogap formation in the doped Hubbard model was first analyzed by the cluster DMFT method (more specifically, Dynamical Cluster Approximation) in Ref. 29. For further applications of the DCA to the 2D Hubbard model, see Refs. 12, 30, 31, 32. In the following consideration, we will not discuss the superconductivity itself, but we will address the so-called Fermi arc phenomenon. Essentially, this is an anisotropic destruction of the Fermi surface in the pseudogap regime. Only the parts of Fermi surface near the nodal direction remain well-defined at low temperature. In the anti-nodal direction, the spectral function at the Fermi level is vanishingly small.

A methodological difference between the doped and the undoped cases is that the sign problem makes direct lattice simulations away from half filling practically impossible. Therefore, the reference point can only be the results of different approximate schemes or the experimental data.

A. Undoped case: translationally-invariant solution

First, we discuss the result of the dual fermion investigation without a spontaneous symmetry breaking which means that the impurity problem is assumed to have no spin-polarization. The data presented in this chapter have been partly discussed previously as a Brief Report.

The translationally-invariant DMFT predicts a Mott transition at rather high value $U > 3.0$ (for a bandwidth $W = 8t = 2.0$). It is important to point out that the density of states at the Fermi energy is independent of $U$ within the entire Fermi-liquid phase. This is a consequence of the locality of the self-energy in DMFT. Therefore, for $U \approx 1.5 - 3.0$, the approximation predicts a three-peak DOS which consists on two Hubbard bands at $\pm U/2$ and a Kondo-like central peak providing the 'pinned' value of DOS at Fermi level.

This behaviour is inconsistent with the reference data described above. Actually, those data do not show a three-peak structure, because of the antiferromagnetic pseudogap. Besides antiferromagnetism, the DMFT sufficiently overestimates the critical value of $U$ for the Mott transition: according to the reference data, the system shows DOS of the Mott-insulator nature already at $U \approx 2.0$ (see Figure 4).

Let us take the leading dual diagram (b) into account. The corresponding data is presented in Figs. 4, 5. Since the self-energy is not local anymore, there is no pinning at Fermi level, and the Kondo-like peak disappears. Furthermore, the self-energy momentum dependence agrees well with the qualitative picture described above. The upper panel of Figure 5 presents contour plots for $\text{Im}\Sigma_{\omega=0,k}$ at $U = 1.0$ and $U = 2.0$ (the data are obtained by a polynomial extrapolation from the Matsubara frequencies). The value of $\text{Im}\Sigma_{\omega=0,k}$ grows dramatically as $U$ changes from 1.0 to 2.0. At larger $U$, there is an expected sharp non-Fermi liquid peak in $\text{Im}\Sigma_{\omega=0,k}$ at Fermi level, without a remarkable anisotropy along Fermi surface. At smaller $U$, the peak is broadened, with maxima near van Hove singularities. The renormalized dispersion law $\epsilon_k + \text{Re}\Sigma_{\omega=0,k}$ is now also in a qualitative agreement with numerical data, as the lower panel of Figure 5. In these graphs, $\epsilon_k + \text{Re}\Sigma_{\omega=0,k}$ is compared with the reference data for a $10 \times 10$ lattice. There is a qualitative difference between the results for $U = 1.0$ and $U = 2.0$: for later case the corrections are quite large so that there is a dependence resembling $\epsilon_k^{-1}$. The superiority of the result against DMFT should be stressed, as there is no $k$-dependence of $\Sigma$ in the DMFT approach.

Let us point out the drawbacks of the present results. First of all, there is still no perfect quantitative agreement with the reference data, although the DMFT result is improved remarkably. The source of this discrepancy becomes clear when the DOS for $U = 1.0$ is plotted (Figure 6). The pseudogap is much narrower in this case. It resembles the situation for $U \rightarrow +0$ at zero temperature, then an antiferromagnetic ordering appears due to long-range nesting phenomena. Its evident from Figure 6 that the calculation with dual diagram (b) does not reproduce this pseudogap at all. Back to the results for $U = 2.0$, the pseudogap in our calculation appears to be not as deep and not as steep, as it should be (Figure 4). We have tried to take higher diagrams into account and found out that it does not help much. We conclude that the dual-fermion corrections, as they considered above, improve the description of short-range Mott physics, but they do not take the long-range antiferromagnetic fluctuations into account.

To explain this failure, let us recall the Hubbard model with small $U$ at zero temperature. As pointed above, our technique passes into weak-coupling diagram expan-
FIG. 5: (color online) Momentum dependence for the self-energy function at Fermi energy, obtained with diagram (b) within the translationally-invariant approximation for the undoped Hubbard model. Data are shown at $t = 0.25, \beta = 20$, for $U = 1.0$ and $U = 2.0$. Upper panel: contour plots for $k$-dependence of the imaginary part of the self energy. Lower panel: renormalized dispersion law $\epsilon_k + \text{Re} \Sigma_\omega$, compared with the reference data obtained for $10 \times 10$ lattice. The Figure has been published previously in the Brief Report 19.

There are two ways to take antiferromagnetism into account. First, one can switch from single-site to cluster DMFT. Thus the antiferromagnetic phase transition maintains the periodical symmetry of the super-lattice made of clusters, there is no problem with non-analyticity in this case. Indeed, various cluster DMFT approaches\textsuperscript{11,12} reproduce the antiferromagnetic gap. The dual-fermion corrections can be used to improve the accuracy of those methods\textsuperscript{35,36}.

The second option is to stay with the single-site starting point, but allow for the antiferromagnetic ordering on the lattice. In this case, the effective impurity problem is spin-polarized. It is known that such an approach indeed works quite well already at the DMFT level\textsuperscript{37}. It can be expected, that the dual-fermion technique can effectively provide the correction in this case. The next section describes such a theory and the corresponding results.

B. Undoped case: antiferromagnetic symmetry breaking

For clarity, let us present the explicit expressions for this case. The antiferromagnetism means that the primitive cell is doubled. The dual Green’s function, as well as other single-electron quantities of the antiferromagnetic state, depends on the difference of the two coordinate arguments and single spin: $G^{\text{dual}}_{\omega,j,s,j',s'} = G^{\text{dual}}_{\omega,j-\mathbf{\Delta},s'}$ (note that $s'$ is defined by $s$ and $r = j - j'$). Given $G^{\text{dual}}_{\omega,r,s}$, it is easy to obtain $\Sigma^{\text{dual}}_{\omega,r,s}$ from the formula (20). In this expression, the spin dependence of $\Sigma$ comes from the spin polarization of $G^{\text{dual}}$ and, in principle, of the vertex $\gamma^{(4)}$. However, the numerical result for the latter quantity appears to be quite noisy. Therefore, we neglected the spin polarization of $\gamma^{(4)}$, performed a averaging over spin orientation, and thus operated with the tensor of the ‘paramagnetic’ symmetry. Such a tensor has the two independent components $\gamma' \equiv \gamma^{(4)}_{s,s}$ and $\gamma'' \equiv \gamma^{(4)}_{s'-s-\bar{s}}$, so that the expression (20) becomes
\[ \Sigma^\text{dual}_{\omega,r,s} = \frac{1}{2\beta^2} \sum_{\omega' + \omega = \omega_1 + \omega_2} \gamma^\prime_{\omega_1\omega_2\omega_3\omega_4} \gamma^\prime_{\omega_1\omega_2\omega_3\omega_4} G^\text{dual}_{\omega_1,r,s} G^\text{dual}_{\omega_2,r,s} G^\text{dual}_{\omega,\omega',r,s} + \frac{1}{\beta^2} \sum_{\omega' + \omega = \omega_1 + \omega_1} \gamma^\prime_{\omega_1\omega_2\omega_3\omega_4} \gamma^\prime_{\omega_1\omega_2\omega_3\omega_4} G^\text{dual}_{\omega_1,r,s} G^\text{dual}_{\omega_2,r,s} G^\text{dual}_{\omega,\omega',r,s} \]

\[ \tag{24} \]

FIG. 7: (color online) Results of DMFT calculation and the scheme with diagram (b), taking the antiferromagnetic ordering into account. The results for local part of the Green’s function at lowest Matsubara frequency are compared with reference data for undoped Hubbard model at \( t = 0.25, \beta = 20 \). QMC calculation at \( 8 \times 8 \) lattice are used for reference.

We believe that this approximation is valid, since the most important contribution to the symmetry-break arises from the spin-polarization of the single electron quantities \( g, \Delta, \) and \( \Sigma^\text{dual} \), entering the expression for \( G^\text{dual} \).

The next step is to write explicitly the definition \( \Sigma^\text{dual} = G^\text{dual} - G^\text{dual(0)} \) in the momentum space. Here, the \( 2 \times 2 \) matrices must be used, as the momentum is conserved up to \( Q = (\pi, \pi) \). Let us denote \( G^\text{dual(0)} = \frac{1}{2}(G_{\omega,j-j',s} + G_{\omega,j-j',-s}) \) and \( G^\text{dual(AF)} = \frac{1}{2}(G_{\omega,j-j',s} - G_{\omega,j-j',-s}) \). It is easy to check that the definition \( \Sigma^\text{dual} = G^\text{dual} - G^\text{dual(0)} \) stays fulfilled with the matrix

\[
\begin{pmatrix} G_k^\text{dual(0)} & G_k^\text{dual(AF)} \\ G_k^\text{dual(AF)} & G_k^\text{dual(0)} \end{pmatrix}
\]

used for \( G^\text{dual} \), and similarly for \( \Sigma^\text{dual}, G^\text{dual} \). This gives a way to construct \( G^\text{dual} \) from a given \( \Sigma^\text{dual} \) and thus close the inner iteration loop. The self-consistency condition (19) remains unchanged, so that the big loop is essentially the same. Finally, the exact relationship (9) can be written in the matrix form, giving thus a complete description of the antiferromagnetic state. Of course, the same treatment with \( \Sigma^\text{dual} = 0 \) corresponds to the antiferromagnetic DMFT.

Actually, once the antiferromagnetism is taken into account, the DMFT result itself already is not too bad. The corresponding data are presented in Figure 7, where we show how the Green’s function at the lowest Matsubara frequency depends on \( U \). At small \( U \), the system is a normal Fermi-liquid. There are small corrections due to the correlations. Of course, DMFT cannot reproduce the anisotropy of the self-energy, but the description of local Green’s function is pretty good. For large \( U \), the system exhibits a strong antiferromagnetism, which is destroyed only at long-range scale. In DMFT, the antiferromagnetic ordering appears in this range. The simplest way to take the long-range fluctuations into account within DMFT framework is to average over the two antiferromagnet sub-lattices. This eliminates the real part of the Green’s function. A comparison of \( \text{Im} G_{\pi/\beta,0} \) with lattice QMC simulations again shows a good agreement (the antiferromagnetic regime starts from \( U \approx 0.85 \), as the inset in Fig.7 shows). The largest deviations of the DMFT result from the reference data occur in the intermediate regime \( U \approx 1 \). Probably, in this regime the fluctuations are essentially non-local but still mid-range. Therefore they cannot be described as a static long-range antiferromagnetic ordering.
The Green's functions are computed with high accuracy, and the maximum-entropy analytical continuation is performed with the same a priori parameters for all curves. This ensures that the graphs for the spectral function can be compared one with another. The spectral function clearly illustrates what is the physical origin of the discrepancy between the DMFT and reference data. Indeed, since DMFT replaces the nonlocal dynamical antiferromagnetic correlations with static ordering, it overestimates the antiferromagnetism in the model. Therefore the pseudogap appears to be too deep; its shoulders and Hubbard bands in the DMFT graph are narrower than they should be. The situation is partly improved for the diagram (b): the shoulders and Hubbard bands are closer to the reference curve although the estimation at Fermi energy looks worse. The serious improvement arises from the next diagram of the ladder, as the dash-dot curve in Figure 9 shows. This is very expectable, because the long-range antiferromagnetic fluctuations are exactly described by these ladders. On the other hand it is interesting to observe from the inset in Figure 9 that this diagram does not improve the result for $G_{\pi}/\beta t=0$, but makes its deviation from the reference data more regular.

C. Doped Hubbard: Fermi arcs formation and flattening of the dispersion law

Here we present the results obtained with the dual-fermion technique for the pseudogap regime, which corresponds to the doping below optimal and relatively high temperature. We use the rotationally-invariant approximation, so the effects of superconductivity and antiferromagnetism were not included in the theory. However it turns out that the theory still captures the physics responsible for the Fermi arc formation, and yields results which compare well to experimental data.

To make the simulation more realistic we introduce the next-neighbor hopping term $t'$. The parameters of the model are $U = 4.0, t = 0.25, t' = -0.075, \beta = 80$. The ratio $t'/t \approx -0.3$ roughly corresponds to the case of YBa$_2$Cu$_3$O$_{y}$[38]. The relatively large value of $U = 2W$ was taken because there is experimental evidence that the system should be a Mott insulator at small doping, which requires $U > 1.5W \approx 3.0$. The temperature used roughly corresponds to 100-150 K, which is a proper value for the pseudogap phenomena in high-temperature superconducting materials. Most of the results are presented on doping level of 14%.

Figure 10 presents the results obtained for the self-energy $\Sigma_{\omega,k}$ at the nodal and anti-nodal points of the Fermi surface. The position of Fermi surface was defined as a maximum of the spectral density. A polynomial extrapolation for $\Sigma_{\omega}$ was constructed to obtain the imaginary part of self-energy at Fermi level. One can observe a remarkable difference in the low-energy limit of $\Sigma_{\omega,k}$ at the nodal and anti-nodal points: the corresponding values of $\text{Im} \Sigma_{\omega=0,k}$ differ approximately by a factor of

![Image of Figure 9](image-url)
FIG. 10: Self-energy function of $tt'$ Hubbard model $\Sigma_{\omega,k}$ at nodal and antinodal points of the Fermi surface at Matsubara frequencies. Diagram (b) is used for the calculations. The data are plotted for 14% doping $tt'$ Hubbard model at $t = 0.25$, $t' = -0.075$, $U = 4.0$, $\beta = 80$. Upper panel: real and imaginary parts of $\Sigma_{\omega,k}$. Lower panel: $\text{Im}\Sigma_{\omega,k}$ in a low-frequency region and its approximation with a 7-th order polynomial.

The spectral function $A_k = (2\pi)^{-1}\text{Im}G_{\omega=0,k}$ for the entire Brillouin zone is mapped in Figure 11 for 14% doping. The Fermi surface in the antinodal direction is quite diffuse, in accordance with the experimental results.

It is worthwhile to consider the spatial dispersion of the self-energy function. The map of $\text{Im}\Sigma_{\omega=0,k}$ is presented in Figure 12, whereas Fig. 13 shows the behavior of this quantity along the $(\pi, \pi) - (\pi, 0) - (0, 0) - (\pi, \pi)$ contour. The data are obtained with a polynomial extrapolation from Matsubara axis. The estimated errorbar of the extrapolation procedure is 0.01. An interesting property of the data obtained is that $\Sigma_{\omega=0,k}$ appears to be substantially non-local, but still short-range. Actually, the data of Figs. 12, 13 can be approximately described by the next-neighbor approximation, that is, the most important components of $\Sigma_{\omega=0,R}$ are $\Sigma_{R=(0,0)}$, $\Sigma_{R=(0,1)}$ and $\Sigma_{R=(1,1)}$. The dotted line in Fig. 13 is produced with these Fourier-components only, and it is quite consistent with the initial curve, except the points $(\pi, 0)$ and $(0, \pi)$ where the self-energy is flattened. It is worth to no-

FIG. 11: Spectral function $A_{\omega=0,k}$ at Fermi level: the calculation with diagram (b) and polynomial extrapolation from Matsubara frequencies. Parameters of the Hubbard model are the same as in Figure 10.

FIG. 12: Imaginary part of the self energy $\text{Im}\Sigma_{\omega=0,k}$ at Fermi level: the calculation with diagram (b) and polynomial extrapolation from Matsubara frequencies. Parameters of the Hubbard model are the same as in Figure 10. The red line indicates Fermi surface.

tice also that $\text{Im}\Sigma_{\omega=0,k}$ is maximal there. Interestingly, variational cluster calculations\textsuperscript{39} demonstrate that near the nodal point, in contrast with the antinodal one, the superconducting gap (that is, anomalous part of the self energy) also can be described in the nearest-neighbor approximation.

Figure 14 shows the effective quasiparticle energy, de-
fined by the formula

$$\epsilon_k^{\text{eff}} = \text{Re} \left[ \frac{\epsilon_k - \mu + \sum_{\omega=0} \omega}{1 + i \frac{\partial}{\partial \omega} \sum_{\omega=0}^{\omega}} \right].$$

(25)

The initial dispersion law $\epsilon_k$ is shown in the same Figure with thin line. One can see an narrowing of the quasiparticle band, mainly due to the $\partial \Sigma_{\omega,k} / \partial \omega$ term. The latter is large due to a closeness to the Mott transition point. Another important change is again the flattening of the curve near $(0, \pi)$ point.

A flattening of the dispersion curve near the antinodal point was earlier predicted as due to a non-Fermi-liquid behavior when the Fermi energy crosses van Hove singularity. The main conclusion of our calculations is that in the strong-interacting regime van Hove point expands to a finite region of the Fermi surface, where the dispersion law is flattened. The $k$-dependence of the self-energy and vertex function are of crucial importance for this phenomenon.

It is worth to note that cluster calculation hardly can reproduce the result for the van Hove behavior, because the flattened region is much smaller than the entire Brillouin zone.

We also performed calculations for other doping. Figure 15 is devoted to $\text{Im} \Sigma$ at 7% doping. Smaller doping makes the system closer to Mott insulator, therefore the value of $\text{Im} \Sigma$ is substantially larger than for the 14% doped system (Figs. 10, 13). The flattened regions disappear in this case. However, there is still a clear difference between the nodal and antinodal directions in the low energy limit: the values of $\text{Im} \Sigma_{\omega=0}$ at these points differ by a factor of two.

Finally, a few words should be said about the region near $(0, 0)$ point in Figure 13, where our polynomial fit predicted slightly positive $\text{Im} \Sigma$ (that corresponds to $\text{Im} G < 0$). We argue here that this is merely an artifact of the extrapolation procedure. Indeed, as it is discussed in section II E, negative $\text{Im} G$ in our theory could only result from a negative residual. However, the graph of $\Sigma$ at Matsubara frequencies for all $k$-points is qualitatively similar to whose shown in the upper panel of Figure 15. It is obvious these graphs have a negative derivative at Fermi energy, so that the residual $Z = (i - \frac{\partial}{\partial \omega})^{-1}$ must be positive.

IV. CONCLUSIONS

To summarize, the transformation to dual fermion variables completely reconstructs perturbation theory, starting with the zeroth-order approximation which is accurate in the limits of both very weak and very strong interactions. As a result, taking into account just a few lower-order diagrams gives quite satisfactory results, without having to resum infinite series of diagrams. Starting with DMFT as the best local approximation, we are able to take into account nonlocal corrections in a regular perturbative way. In contrast with several cluster approaches the method is exactly translationally invariant and allows us to analyze how different parts of the reciprocal space are distinctly affected by correlation effects.

This approach can be setup either in phases with long-range order (antiferromagnetism, superconductivity) or in phases without long-range order (normal state) by not allowing for symmetry breaking. The present article mostly deals with the latter case. By doing so, we could focus on physical effects that are not directly related to incipient long-range order. In particular, we...
showed that the anisotropic destruction of quasiparticles and the Fermi surface (at least, as presented in Figs. 10–14) is not due to precursor effects of antiferromagnetism (or superconductivity) as soon as the intermediate and strong coupling regimes are entered. Indeed, it is associated with quite-short range physics, as illustrated by the fact that only the short-range components of the self-energy are found to have significant magnitude. This observation also provides some support to cluster extensions of DMFT.

Although the destruction of quasiparticles in a momentum-selective way is adequately captured by this approach and associated with short-range correlations, more work is required (possibly including symmetry breaking and incipient long-range order) in order to reach a proper description of the pseudogap formation and of its dependence on the doping level and on the $t'/t$ ratio.

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APPENDIX A: EXACT RELATIONS FOR HIGH-ORDER CUMULANTS

Similarly to the exact relationship (9) between the initial and dual Green’s function, the one-to-one correspondence between higher-order momenta for the initial and dual system can be established. Particularly, the formula for the four-order Green’s function was presented and discussed previously. It was shown that the two-particle excitations in the original and dual system are identical. Here, we use the generating functional approach, that allows us to establish the general structure of such relationships for high momenta, and extend the conclusion about the two-particle excitations to all collective excitations, involving an arbitrary number of particles.

We start from the expression for action (8), which includes both initial and dual variables. Then we introduce the independent variations of initial and dual energy:

$$S[c, c^*, f, f^*; u, v] = S[c, c^*, f, f^*] + u_{12} c_1^* c_2 + v_{12} f_1^* f_2,$$

where $u$ and $v$ are infinitesimal and a summation over repeating indices is implied.

One can see that Taylor series of the functional

$$F[u, v] = \ln \int e^{-S[c, c^*, f, f^*; u, v]} DcDc^* DfDf^*$$

with powers of $u$ and $v$ correspond, respectively, to the cumulants of initial and dual system. We remind that the second-order cumulant is the Green’s function, and higher-order cumulants are proportional to corresponding vertex parts. For example, the fourth-order cumulant

$$\frac{\partial^2 F}{\partial u \partial v} = X_{1234} - G_{23} G_{14} + G_{13} G_{24}$$

($X$ is the two-particle Green’s function), whereas the fourth-order vertex

$$\Gamma^{(4)}_{1234} = G_{11}^{-1} G_{22}^{-1} \frac{\partial^2 F}{\partial u \partial v} G_{33}^{-1} G_{44}^{-1}.$$

To establish a relation between the cumulants, let us integrate over $f^*$, $f$ in the previous formula. We obtain

$$F[u, v] = F_0[u, v] + \ln \int e^{-S[c, c^*; u, v]} DcDc^*$$

and

$$F_0[u, v] = -\ln \det |1 + (\Delta - \epsilon) \alpha^{-1} v \alpha^{-1}||$$

where $u$ and $v$ are infinitesimal and a summation over repeating indices is implied.

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and

$$F_0[u, v] = -\ln \det |1 + (\Delta - \epsilon) \alpha^{-1} v \alpha^{-1}||$$

where $u$ and $v$ are infinitesimal and a summation over repeating indices is implied.

Let us consider the fourth-order cumulants

$$\frac{\partial^2 F}{\partial u \partial v}$$

and

$$\frac{\partial^2 F}{\partial u \partial v}.$$
cumulants vanish due to the Fermi-operator algebra. For the case of different indices, the differentiation is quite simple and gives, after putting $\alpha = g^{-1}$, formula (29) of the paper 35.

$$\frac{\delta^2 F}{\partial u_{32} \partial u_{41}} = L_{11}' L_{22}' \frac{\delta^2 F}{\partial v_{32}' \partial v_{41}'} R_{33}' R_{44}' .$$ (A4)

Here $L$ and $R$ are matrix inverse of $(\Delta - \epsilon)^{-1} g$ and $g(\Delta - \epsilon)^{-1}$, respectively. It should be emphasized that this expression does not contain any extra additive terms, in contrast to formula (9). Formally this is because the second derivative $\frac{\delta^2 F_0}{\partial u_{32} \partial u_{41}}$ vanish, as one can check straightforwardly. Physically this means that the two-particle excitations in the original and dual system are identical.\(^\dagger\)

There might be also instructive to re-express the last formula in terms of vertex function. Putting also $\alpha = g^{-1}$, one obtains

$$\Gamma_{1234} = L_{11}' L_{22}' T^{dual}_{1234} P_{33}' P_{44}' ,$$ (A5)

where $\Gamma' = (1 + \Sigma_{dual}(g)^{-1}$ and $P' = (1 + g \Sigma_{dual})^{-1}$.

One can see that the obtained formulas are formally valid also for the case of coinciding indices, when both left- and right-hand sides vanish.

An advantage of the presented approach is that the derivation of the formulas for six and higher-order vertex parts appears to be literally the same as for the fourth order. All the argumentation about the absence of the coinciding indices and vanishing of the high derivatives of $F_0$ is valid for that case. Therefore formula (A5) is valid for vertex parts of any order, just a number of indices and multipliers $L'$, $R'$ should be changed. From the physical point of view, we conclude that all collective excitations of the initial and dual ensemble are the same.

**APPENDIX B: FUNCTIONAL MINIMIZATION, RELATION TO DMFT, AND SELF-CONSISTENCY CONDITION**

It is clear from the present consideration that a proper choice of the hybridization function $\Delta$ is crucial. A functional-minimization scheme is suitable to clarify this issue. Let us introduce a trial action $\tilde{S}[f, f^*]$. For clarity, we put the subscript $\tilde{S}$ at the triangle brackets in this section, to emphasize the the averaging is over the system with trial action $\tilde{S}$. We consider Feynman’s variational functional

$$< \tilde{S} >_{\tilde{S}} + \ln \int e^{-\tilde{S}DfDf^*} - < S >_{\tilde{S}} - \ln \int e^{-S DfDf^*} = \max .$$ (B1)

A straightforward variation $\tilde{S} \to \tilde{S} + \delta S$ gives an extremum condition

$$< (S - \tilde{S}) \delta S >_{\tilde{S}} = < (S - \tilde{S}) >_{\tilde{S}} < \delta S >_{\tilde{S}} .$$ (B2)

For an arbitrary $\delta S$, this indeed means that the extremum of (B1) is delivered by $\tilde{S} = S$, up to an additive constant. In this case (B1) vanishes. The larger value of (B1) corresponds to the better approximation.

There is an important point: since dual action depends on $\Delta$, the condition (B1) can be used to determine the optimal $\Delta$. The variation with respect to $\Delta$ gives

$$\frac{\delta < S >}{\delta \Delta} = 0 .$$ (B3)

Here we took into account that variations of $\tilde{S}$ and $\Delta$ are independent, so the first two terms of (B1) do not vary with $\Delta$. As for the last term, it is exactly $\ln Z$ and therefore independent of $\Delta$ as well.

Now, recalling $S[f, f^*] = - \ln \int e^{-S[c, c^*, f, f^*]}$ and substituting (8), we obtain after certain transformations that (B3) corresponds to the condition

$$G_{\omega, r=0} = g^{imp}[f, f^*] > \tilde{S} ,$$

$$g^{imp}[f, f^*] = \frac{\int e^{-S_{site} + \tilde{S}_{site} + \tilde{S}_{imp}DfDf^*} \int e^{-S_{dual}DfDf^*} \int e^{-S_{dual}DfDf^*} d\omega_i d\omega_j d\omega_k} {Z} .$$ (B4)

Here $S_{site}$ is defined by formula (10) and $G_{r=0} = N^{-1} \sum_k G_k$ is local part of the Green’s function. While deriving these formulas, it is useful to take into account that $\alpha = g^{-1}$ is just a scaling factor standing at $f^*, f$, and there is no need to vary this quantity: one can vary with respect to $\Delta$ at fixed $\alpha$ and put $\alpha = g^{-1}$ afterwards.

Actually, the criterion (B4) has a very clear meaning: local part of the Green’s function equals the Green’s function of the single-site action $S_{site}$, averaged over the fluctuations of $f$. Neglecting these fluctuations, one obtains just a DMFT condition for hybridization function, that is $G_{\omega, r=0} = g_{\omega}$.

To make the consideration more clear, let us first consider the Gaussian approximation for dual variables, $\tilde{S} = -g_{dual}^{-1} f f^*$. Let us show for this Gaussian trial action, the DMFT condition

$$G_{\omega, r=0} = g_{\omega}$$ (B5)

satisfies (B4) exactly (call this statement T1). The proof is based on the observation that the condition (B5) is equivalent to the requirement that the local part of dual Green’s function equals zero,

$$G_{r=0}^{dual} = 0 ,$$ (B6)

as one can easily check with formulas (14, 15). Further, since $\tilde{S}$ is Gaussian, formula (B6) means that all local momenta $< f_i f_i >$, $< f_i f_i f_i >$, $< f_i f_i f_i f_i >$, ... equal zero. It means that local fluctuations of $f, f^*$ are virtually absent, therefore $g^{imp}[f, f^*] = g_{\omega}$ and (B4) becomes (B5). To obtain a formal proof, one should consider an average of the Taylor series for $g^{imp}[f, f^*]$. These series starts from $g_{\omega}$, whereas the average of any higher term vanishes. This proves T1.
Next, it is possible also to show that the DMFT Green’s function is optimal with respect to the variations of the Gaussian trial action (call this statement T2). With a variation $\tilde{S} = -\mathcal{G}^{-1}_{dual} f^* f \rightarrow \tilde{S} = -\mathcal{G}^{-1}_{dual} f^* f + 0f^*_i f_j$, formula (B2) becomes

$$\langle (S + \mathcal{G}^{-1}_{dual} f^* f) f^*_i f_j \rangle = \langle S + \mathcal{G}^{-1}_{dual} f^* f \rangle = \langle f^*_i f_j \rangle .$$

The essential point is again that since all local momenta of $f, f^*$ are vanished because of (B6), and the dual potential $V$ is local in space, all the nonlinearity drops out from the (B7). It means that both left- and right-hand sides of (B7) equal the same value, if $-\mathcal{G}^{-1}_{dual} f^* f$ equals the Gaussian part of the dual action. This proofs T2.

So, we have shown that the DMFT procedure can be considered as the Gaussian approximation for the dual variables, which is optimal in sense of Feynman minimization criterion, with respect to both trial action and hybridization function.

Beyond the Gaussian trial action, an analytical treatment of the extremal criterion (B1) is hardly possible. Therefore, in the main body of the theory we treat the dual system perturbatively, using the diagram series with respect to $V$ and the hybridization function defined from the condition (19).

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