Josephson lattice model for phase fluctuations of local pairs in copper-oxide superconductors

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We derive an expression for the effective Josephson coupling from the microscopic Hubbard model. It serves as a starting point for the description of phase fluctuations of local Cooper pairs in d_{x^2−y^2}-wave superconductors in the framework of the XY-model. The interaction is derived by means of the local-force theorem and depends on local correlation functions, that we obtain by the cluster dynamical mean-field theory. We compare predicted London penetration depths and Kosterlitz-Thouless transition temperatures with experimental data of YBa$_2$Cu$_3$O$_7$.

Despite a lot of attempts a commonly recognized theory of High- $\mathrm{T}_c$ superconductivity[1–9] doesn’t exist yet. Most of the theoreticians believe that the basic physics is connected with the correlations in the subsystem of copper d-electrons and can be understood, in its main features, in the framework of the Hubbard model. However, it remains debatable whether superconductivity can exist because of interelectron interaction via spin fluctuations[3] or because of interlayer tunneling[10].

One of the most important experimental data concerning these problems is the existence of a pseudogap[11] in the electron density of states above the critical temperature. However, the nature of the pseudogap is highly debated: it can be attributed either to antiferromagnetic-like spin fluctuations or to local pairs. The situation is still non-transparent both experimentally and theoretically.[12–15] However, the cuprates show properties of highly correlated systems[16], in which a broad circle of phenomena have been studied by the dynamical mean-field theory (DMFT)[17]. Since d-wave superconductivity (dSC) exists between sites, one has to use a cluster version of DMFT (CDMFT).[15, 18–27]

We proceed with the Hubbard model[28, 29]

$$H = \sum_{k\sigma} t(k)c_{k\sigma}^\dagger c_{k\sigma} + U \sum_r n_{r\uparrow} n_{r\downarrow},$$

(1)

where $t(k)$ are the Fourier-transformed hopping parameters, $U$ is the interelectron Coulomb repulsion parameter on site $r$ and $n_{r\sigma} = c_{r\sigma}^\dagger c_{r\sigma}$, $c_{r\sigma}^\dagger$, $c_{r\sigma}$ are electron creation and annihilation operators in site (momentum) representation. Regarding the CuO$_2$ plane, we use nearest neighbor hopping $|t|$ as the energy unit, the next-nearest neighbor hopping $t'/t = −0.3[30]$ and the nearest neighbor interlayer hopping $t_{\perp}/t = 0.15[31]$. For the screened Coulomb interaction we choose $U = W = 8$, that is the same value as for the bandwidth $W$. We consider the 2D square lattice ($t_{\perp} = 0$) and 3D cubic lattice cases. The Brillouin zone has been normalized to 1 for all dimensions. For a comparison with experimental data we use the factors $a_0/2, a_b/2, a_c = 3.82\text{Å}, 3.82\text{Å}, 3.89\text{Å}$

to restore the physical dimensions according to the distances of the Cu-atoms in YBa$_2$Cu$_3$O$_7$[32, 33] (YBCO), neglecting the different interlayer distances. Furthermore it has the superexchange $t = 0.35\text{eV}$.

We use Anderson’s pseudospin description of superconductivity[34]. For our specific problem it means that we consider the order parameter of dSC pairing as an analog of the local magnetic moment and investigate macroscopic coherence as a result of (“exchange”) interactions between plaquettes (see Fig. 1), similar to the description of magnetic ordering in terms of an effective Heisenberg Hamiltonian[35, 36]. The superconducting phase ordering can be described in terms of an effective Josephson Hamiltonian

$$H_{\text{eff}} = - \sum_{ij} J_{ij} \cos(\theta_i - \theta_j),$$

(2)

where $i, j$ are plaquette indices, because we use the CDMFT[37, 38] approach in that the cluster self-energy does only exist on the cluster and not between clusters.[19–21, 23–26] For this purpose, we consider the elementary plaquette in the Cu layer as a supersite and introduce a superspinor $C_i^\dagger = (c_i^\dagger, c_i^\dagger, c_i^\dagger)$ where $i$ is the index.

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\[ \Sigma_i, \Sigma_j \]

**FIG. 1.** Illustration of the Hubbard-plaquette lattice ($t, U$) with lattice vector $r$ and local self-energies $\Sigma_i$. It is mapped to the XY-model with effective Josephson coupling $J_{ij}$ of plaquettes due to phase fluctuations $\delta \theta_i$ of the superconducting gap $\Delta$. 

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of the plaquette and α = 0, 1, 2, 3 labels the sites within the plaquette. In order to describe the superconducting state we use a Gor’kov-Nambu spinor representation for the Green function which is a 2x2 matrix. Thus the full lattice Green function \( G_{ij} \) is an 8 x 8 matrix.

To obtain explicit microscopic expressions for the Josephson coupling parameters \( J_{ij} \) we calculate the microscopic variation of the thermodynamic potential \( \Omega \) of the system under small variations of the phases and compare the result with that from Eq. (2). It depends on the lattice Green function that we can substitute via the Dyson equation by the local self-energy of CDMFT

\[
\left( \begin{array}{cc} G^\rho \rho & F \\ F & G^h \h \end{array} \right)^{-1}_{ij} = \left( \begin{array}{cc} G^\rho_0 \rho & G^h \h_0 \\ G^h_0 & G^\rho \rho \end{array} \right)^{-1}_{ij} - \delta_{ij} \left( \begin{array}{cc} \Sigma^\rho \rho & S \\ S & \Sigma^h \h \end{array} \right) ,
\]

(3)

The superscripts \( \rho \) and \( h \) denote particle and hole, respectively. They are related by \( G^\rho (i\omega) = - (G^h (i\omega))^\ast \). The anomalous (off-diagonal) parts of the self-energy (S) and Green function (F) describe dSC pairing in the plaquette and are matrices in plaquette sites (\( \alpha \)) with non-zero elements \( S_{01} = - S_{12} = S_{32} = - S_{03} \). Furthermore, we consider finite temperatures and therefore the correlation functions depend on fermionic Matsubara frequencies.

Then the local-force theorem[36] gives

\[
\delta \Omega = \text{Tr} \ln (1 - G \delta^\ast \Sigma) ,
\]

(4)
in that \( \delta^\ast \) is the local variation of the self-energy without taking into account its variation due to the DMFT self-consistency and \( G \) is the lattice Green function without variation. Eq. (4) is rigorous in the first order of \( \delta \).[36] However, we will use it also for the second order terms. It corresponds to neglecting vertex corrections, that is reasonable to assume for the ordered phase.[39, 40] Near the transition we believe that it can be used at least for the estimation of parameters of the superconducting state.

For our specific problem we design the variation as an infinitesimal change of the (plaquette-)local phase \( \delta \theta_i \), for that holds \( \theta^h = - \theta^\rho \). Therefore it reads

\[
\delta^\ast \Sigma_i = e^{i \delta \theta_i} \sigma_z / 2 \Sigma_i e^{-i \delta \theta_i} \sigma_z / 2 - \Sigma_i ,
\]

(5)
in that the third Pauli matrix \( \sigma_z \) acts on the Nambu-space. It is a \( U(1) \)-rotation of the local self-energy that changes only the anomalous parts. \( \Sigma_i \) is the numerical[41, 42] solution of the CDMFT (Eq. (3)) using the continuous-time quantum Monte-Carlo (CTQMC) method, see supplemental material[43] for details. Eq. (4) and Eq. (5) lead to the following expression for the Josephson lattice parameters[43]

\[
J_{ij} = T \text{Tr}_{\omega \alpha} \left( \begin{array}{cc} F_{ij} S_{ij} F_{ij} S_{ij} - G^\rho_{ij} S_{ij} G^h_{ij} S_{ij} \end{array} \right) ,
\]

(6)

Its structure is similar to the expression for the magnetic interactions.[36]

To consider the thermodynamics of the “Josephson lattice” model of Eq. (2) it is important to go to a continuum limit with the integration over the volume \( d^dr \)

\[
H_{\text{eff}} = \frac{1}{2} \sum_{ab} I_{ab} \int d^dr \frac{\partial \theta}{\partial r_a} \frac{\partial \theta}{\partial r_b} ,
\]

(7)

where \( a, b \) are Cartesian indices, \( I_{ab} \) is the stiffness matrix and \( r \) are position vectors in the plaquette-continuum. Substituting Eq. (6) into \( I_{ab} \) and passing to the momentum representation[43] we obtain

\[
I_{ab} = \frac{T}{(2\pi)^3} \int d^dr Tr_{\omega \alpha} \left( \begin{array}{cc} \langle \partial F(k) \rangle & \partial F(k) \rangle S - \langle \partial G^\rho(k) \rangle \frac{\partial S}{\partial k_a} \langle \partial G^h(k) \rangle \frac{\partial S}{\partial k_b} \end{array} \right) ,
\]

(8)

here \( k \) is a wave vector in the reduced Brillouin zone space. For our model the stiffness matrix is diagonal \( ||I_{ab}|| = \text{diag} (I_{||}, I_{||}, I_{⊥}) \) with the in-plane component \( I_{||} \) and the perpendicular component \( I_{⊥} \).

The temperature dependence of the dSC stiffness can be divided into two qualitatively different regions, see Fig. 2 (top). For \( 0 < \delta \lesssim 0.075 \) the temperature, at that \( I_{||} \) becomes non-zero, is constant. \( I_{||} \) saturates quickly with decreasing \( T \) and the maximum within the considered temperature range \( (0.02 \lesssim T \lesssim 0.06) \) grows. It is, for \( 0.075 \lesssim \delta \lesssim 0.15 \) the temperature of non-zero \( I_{||} \) as well as the maximum value of \( I_{||} \) decrease. Characteristics of the latter have been found in YBCO (and \( La_{2-x}Sr_xCuO_4 \)[44]) with a constant slope \( I_{||} (T) \) for different underdopings[45, 46] and also in a study of the intensity of a current-current correlation function’s Drude-like peak[20]. Note that the latter method can give just a number for the superfluid density whereas our approach allows to restore the whole Hamiltonian with the non-local effective Josephson parameters.
The temperature dependence looks very similar to that of the order parameter of local Cooper-pair formation, see Fig. 2 (bottom), that is defined as
\[ \Phi_{\text{SC}}^{\text{CDMFT}} = \langle c_{\uparrow X} c_{\downarrow X} \rangle = -\langle c_{\uparrow Y} c_{\downarrow Y} \rangle \] (9)
where we performed a unitary transformation on the intra-cluster sites into the plaquette-orbital basis, that can be regarded as a discrete Fourier transform and hence the orbital labels \( \Gamma, X, Y \) and \( M \). Thus the main effect stems from the absence of local Cooper-pairs. The most prominent difference between \( I_\parallel \) and \( \Phi_{\text{SC}}^{\text{CDMFT}} \) in the saturation at low temperatures, especially in the underdoped region. Regarding the accuracy of the local-force theorem it is important to check whether the saturation of the local order parameter \( \Phi_{\text{SC}}^{\text{CDMFT}} \) with respect to decreasing temperature is reached. Otherwise amplitude fluctuations of the dSC gap may play a stronger role and vertex corrections become significant.[39] Our calculations show a saturation at \( T \sim 0.02 \) for dopings \( \delta \lesssim 0.1 \). Arbitrary low temperatures for the \( I_\parallel (T = 0) \)-estimate, that we will discuss below, can not be reached because of the CTQMC-fermionic sign problem.[15]

So far we have only discussed the 2D lattice. In Fig. 3 we compare the in-plane/perpendicular dSC stiffness and penetration depth as well as the order parameter of local Cooper pair formation for different \( t_\parallel \) and \( t' \). \( t_\parallel \) has a minor impact on \( I_\parallel \), in contrast \( t' \) reduces it significantly (Fig. 3, top). Remarkably, for small dopings \( \delta < 0.05 \) \( I_\parallel \) is rather independent of \( t_\parallel \) and \( t' \). Then for larger dopings \( I_\parallel \) of \( t' = 0.3 \) has a symmetric dome shape, whereas for \( t' = 0 \) it is skewed with a more pronounced maximum at larger dopings. \( I_\parallel \) is an order of magnitude larger than \( I_\perp \) (Fig. 3, center) reflecting the fact that for the Josephson lattice model the superfluid is still more concentrated within the strongly coupled CuO planes rather than in between. A comparison with the order parameter \( \Phi_{\text{CDMFT}}^{\text{SC}} \) (Fig. 3, bottom) reveals that their respective maxima do not coincide and their profile is very different.

The superconducting stiffness is closely related to the London penetration depth \( \lambda \), namely
\[ \lambda_{ab/c}^2 = \frac{1}{\hbar c} I_{1/\perp}. \] (10)

The penetration depths have been measured in several experiments close to optimal doping. The zero-temperature values lie in the range of \( \lambda_a = 100\text{nm} - 160\text{nm} \) and \( \lambda_c = 635\text{nm} \).[47, 48] Finite temperature corrections can add \( \Delta \lambda_{ab}(T = 80K) \sim 100\text{nm} \).[49] The largest parallel penetration depth that we found for \( t' = 0.3 \) is \( \lambda_{ab} = 110\text{nm} \). This value corresponds to a doping at that the temperature-dependent saturation of the stiffness has been reached (Fig. 2) and we can compare it to zero-temperature measurements. Therefore it matches well into the series of measurements. Additionally we found \( \lambda_c \sim 700\text{nm} \), that is within 10% of the measured zero-temperature value.

In the 2D case the model of Eq. (2) exhibits the Kosterlitz-Thouless (KT) transition, that corresponds to the unbinding of vortex-antivortex pairs. The transition temperature is
\[ T_{KT} = \frac{\pi}{2} I_{1/\parallel}. \] (11)

At \( T < T_{KT} \) there is no real long-range order in the system but power-law decay of the correlation function of the superconducting order parameter. In this sense interlayer tunneling is essentially important to have long-range order, i.e. real superconductivity at macroscopic scales.

In Fig. 4 we present the transition temperatures of CDMFT \( T_c^{\text{CDMFT}} \) and of the Kosterlitz-Thouless transition \( T_{KT} \). \( T_c^{\text{CDMFT}} \) has been calculated using a Mean-field fit and \( T_{KT} \) from the superconducting stiffness according to Eq. (11). It is an estimate as we use the stiffness of \( T \sim 0.02 \) throughout in order to calculate the transition temperature. The solid line of the Kosterlitz-Thouless transition \( T_{KT} \) is the part of the phase diagram in that the low-temperature saturation of \( \Phi_{\text{SC}}^{\text{CDMFT}} \) and \( I_\parallel \) has been reached and thus the application of our method reliable. For the dotted line part amplitude fluctuations can change the transition temperature.

Superconductivity is strongest suppressed by phase fluctuations at small dopings. This is where local Cooper-pairs according to CDMFT are well pronounced. Note that local antiferromagnetic fluctuations are respected by our method, but long-ranged spin waves are not. Both can contribute to the suppression of superconductivity in \( \delta \lesssim 0.05 \) in cuprates.[11] The maximum transition
We thank G. Homann and L. Mathey for discussions on applications of effective Josephson couplings and models.

The optimal value for the doping of the CuO planes is $\delta = 0.15$, that is within the region that requires CDMFT calculations with $T < 0.02$ in order to neglect vertex corrections.

Our theory provides a connection from the Hubbard model to effective theories of the Josephson coupling only. Those have been applied to investigate experiments in that interplane Josephson coupling has an essential role. We present a selection of the Josephson couplings of the parallel and perpendicular plaquette-translations in Fig. 5. $J_r$ decreases rapidly with increasing plaquette-translation length $|r|$ and the short-range components of $J_r$ alone can give a complete description.

We find that effective Josephson models with a nearest neighbor coupling $J_{(1,0,0)}$ only are reasonable for $t' = 0.3$ as it is an order of magnitude larger than the remaining couplings $J_r$ (Fig. 5, left). In contrast, for $t' = 0$ and $\delta \sim 0.1$ the next-nearest neighbor coupling $J_{(1,1,0)}$ has the same order of magnitude and should be treated accordingly. The second- and third-nearest neighbor Josephson couplings $J_{(1,1,0)}$ and $J_{(2,0,0)}$ are split by up to one order of magnitude for $t' = 0$. In opposite, with $t' = 0.3$ the two are competing and intersect close to $\delta = 0.12$.

The interplane coupling $J_{(0,0,1)}$ is an order of magnitude smaller than $J_{(1,0,0)}$ and $t'$ can change its doping dependence qualitatively. Those effects will be interesting to study further within the XY-model, e.g. in the context of La$_{2-x}$Ba$_x$CuO$_4$.

An increase of the interlayer hopping $t_\perp$ increases the interplane Josephson coupling sharply ($\Delta J_{(0,0,1)}/\Delta t_\perp \sim -10^2$) at small hole-dopings (Fig. 5, right). On the other hand the in-plane Josephson couplings are rather constant as functions of $t_\perp$. It turns out that $J_{(1,1,0)}$, $J_{(2,0,0)}$ and $J_{(0,0,1)}$ have very similar values around our considered realistic $t_\perp = -0.15$.

In conclusion, based on the local-force theorem we have derived a mapping from local correlation functions of the Hubbard model, obtained by CDMFT, to an effective Josephson coupling. We have introduced local $U(1)$-phase fluctuations in the thermodynamic potential and mapped it to the XY-model to describe the role of phase coherence of the Cooper-pairs in the cuprates. The dSC stiffness is calculated for the thermodynamic limit of the XY-model at low temperatures. We have found that its profile for underdopings is strongly suppressed compared to the order parameter of local Cooper-pair formation. The penetration depths calculated from the dSC stiffness ($\lambda_{ab} = 110$nm, $\lambda_c = 700$nm) give reasonable estimates in comparison with experimental data of YBCO.

The temperature of the Kosterlitz-Thouless transition of the 2D XY-model at small hole-dopings is smaller than the critical temperature of local Cooper-pair formation. The maximum of the former ($T_{KT}^{\max} \sim 120$K) is about one third smaller than the maximum of the latter ($T_{c}^{\text{CDMFT, max}} \sim 180$K), which is closer to the transition temperature of YBCO and especially close to the upper bound of the Nernst-region. For small hole-dopings ($\delta \leq 0.05$) $J_{(1,0,0)}$ is much larger than the remaining couplings. However, this changes for larger dopings and also depends on the hopping parameters.

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I. LOCAL-FORCE THEOREM FOR SUPERCONDUCTIVITY

We present the details of the derivation of the Josephson coupling $J$ and start with a generic outline of the local-force theorem[1] before we get more specific about the $d$-wave superconductivity (dSC) setup.

The starting point is the free energy functional

$$
\Omega = \Omega_{sp} - \Omega_{dc},
$$

$$
\Omega_{sp} = - \text{Tr} \ln (-G^{-1}),
$$

$$
\Omega_{dc} = \text{Tr} \Sigma G - \Phi,
$$

where the free energy is split into the single-particle $\Omega_{sp}$ and the double-counted $\Omega_{dc}$ parts, labeled in analogy to the density functional theory. The single-particle term depends on the lattice Green function $G$. $\Phi$ is the Luttinger-Ward generating functional[2] (sum of all the skeleton diagrams without free legs).

Regarding the Green function as the resolvent we can perform the perturbation on the system as

$$
\delta^{*}G^{-1} = -\delta^{*}\Sigma. \tag{3}
$$

and thereby for the total variation of the free energy we obtain

$$
\delta \Omega = \text{Tr} \ln (1 - G^{*} \Sigma). \tag{4}
$$

The variation is specified further by writing the locality of the self-energy explicitly $\Sigma_{ij} = \delta_{ij} \Sigma_i$. However, the expansion of the (matrix-)logarithm, in that different sites are coupled by $G_0$, has non-local effects

$$
\delta \Omega = \sum_{ij} \text{Tr} \left( \delta_{ij} G_{ij} \delta^{*} \Sigma_i + \frac{1}{2} G_{ij} \delta^{*} \Sigma_j G_{ji} \delta^{*} \Sigma_i \right). \tag{5}
$$

I. LOCAL-FORCE THEOREM FOR SUPERCONDUCTIVITY

The trace goes over all degrees of freedom except for $i, j$.

At this point we need to specify the basis and perturbation according to our setup and superconductivity. The local self-energy is a solution of the cluster dynamical mean-field theory (CDMFT), where the self-energy exists only within a plaquette, that can be considered as a supersite. The change, that we apply to the system is a $U(1)$ rotation in Nambu-space. It corresponds to a change in the phase of the plaquette-local superfluid. Therefore $i, j$ are plaquettes and the trace of Eq. (5) goes over Matsubara frequencies $\omega$, plaquette-sites $\alpha$ and Nambu-space. The Nambu space is used to make the perturbation explicit, we use the generator of finite rotations in it,

$$
\delta^{*} \Sigma_i = e^{i \delta \theta_i \sigma_z / 2} \delta^{*} \Sigma_i e^{-i \delta \theta_i \sigma_z / 2} - \Sigma_i \tag{6}
$$

$$
= \left( \begin{array}{cc} \Sigma_{ii}^p & e^{i \delta \theta_i} \Sigma_{ij}^h \\ e^{-i \delta \theta_i} \Sigma_{ji}^h & \Sigma_{jj}^p \end{array} \right) - \Sigma_i \tag{7}
$$

$$
\approx \left( \begin{array}{cc} 0 & (i \delta \theta_i - \frac{(\delta \theta_i)^2}{2}) \Sigma_{ii}^h \\ -i \delta \theta_i - \frac{(\delta \theta_i)^2}{2} & 0 \end{array} \right), \tag{8}
$$

that we insert into both terms of Eq. (5)

$$
G_{ij} \delta^{*} \Sigma_i =
$$

$$
\left( F_{ij} S_i \left( -i \delta \theta_i - \frac{(\delta \theta_i)^2}{2} \right) G_{ji}^p S_j + G_{ij}^h S_i \left( i \delta \theta_i - \frac{(\delta \theta_i)^2}{2} \right) \right) \tag{9}
$$

$$
G_{ij} \delta^{*} \Sigma_i G_{ji} \delta^{*} \Sigma_j =
$$

$$
\left( -F_{ij} S_j F_{ij} S_i + G_{ij}^p S_j G_{ji}^h S_i \right) \tag{10}
$$

We keep terms up to second order in $\delta \theta$ and since we are interested in the trace we omit off-diagonals in Eq. (10).

Note, that in analogy to the $SU(2)$-rotations of local magnetic moments it is reasonable to assume that the neglect of vertex corrections in second order gives accurate estimates, if the local order parameter of our $U(1)$-rotors are well pronounced, which is typically the case at sufficiently low temperatures. It is in accordance with the idea of describing the low-energy modes of the system by the $XY$-model, in that amplitude fluctuations of the dSC gap are absent.
Using $\delta \theta_{ij} \equiv (\delta \theta_i - \delta \theta_j)$ and
\begin{equation}
2 \delta \theta_{i} \delta \theta_{j} = - \delta \theta_{ij}^2 + \delta \theta_{i}^2 + \delta \theta_{j}^2 \tag{11}
\end{equation}
we can execute the trace on the Nambu space and sort the terms by their order in $\delta \theta$,
\begin{equation}
\delta \Omega = \sum_{i,j} Tr_{\omega \alpha} \left( G_{ij}^{\dagger} S_j G_{ji}^{\dagger} S_i - \delta \theta_{ij} F_{ji} S_i - F_{ij} S_j F_{ji} S_i \right) \delta \theta_{i}^2 \\
+ \frac{1}{2} \sum_{i,j} Tr_{\omega \alpha} \left( F_{ij} S_j F_{ji} S_i - G_{ij}^{\dagger} S_j G_{ji}^{\dagger} S_i \right) \delta \theta_{ij}^2.
\tag{12}
\end{equation}
We still have the trace over the sites within the plaquette and the products are matrix products in that space. For the Matsubara frequencies this is not particularly interesting as the correlation functions are diagonal on those. In order to obtain Eq. (12) we have also used the cyclic property of the trace and the lattice symmetry $G_{ij} = G_{ji}$.

The term $\propto \delta \theta_i^2$ vanishes (see Sec. II, below) and reflects the gauge invariance of the theory. We are left with only non-local phase fluctuations, that are $\propto \delta \theta_{ij}^2$:
\begin{equation}
\delta \Omega \equiv \frac{1}{2} \sum_{i,j} J_{ij} \delta \theta_{ij}^2
\tag{13}
\end{equation}
and make it as the defining equation for $J_{ij}$,
\begin{equation}
J_{ij} = T Tr_{\omega \alpha} \left( F_{ij} S_j F_{ji} S_i - G_{ij}^{\dagger} S_j G_{ji}^{\dagger} S_i \right). \tag{14}
\end{equation}
We interpret this variation as a model of its own. The minimization with respect to a $U(1)$-phase is described by the $XY$ model
\begin{equation}
H = - \sum_{i,j} J_{ij} \cos \theta_{ij}.
\tag{15}
\end{equation}
The $XY$ model originally has been applied to the problem of classical spins that minimize their energy by adjusting their relative angle ($U(1)$). But we describe here the long-range coherence of Cooper pairs. Hence it is called the Josephson lattice model.

Fig. 1 shows the doping dependent coupling and its contributions by the two terms of Eq. (14). $J$ obviously can only take on finite values if there is a superconducting gap and therefore a finite anomalous self-energy $S$. The nearest neighbour Josephson coupling $J_{(1,0,0)}$ consists mainly of the second term, that is 3 times as large as the first. At $\delta \sim 0.07$ the first term vanishes. The second and third in-plane nearest neighbors have contributions from both terms and they are of similar magnitude. However, the doping dependence has features, i.e. A local minimum of the second term appears, at a point where the first term has a maximum.

II. SUM RULE

Sum-rules express correlations of certain transitions in terms of sums over other transitions. We derive a set of sum-rules starting from the Dyson equation. In this section we work in the Nambu-space (omitting the spin labels for convenience), but the quantities can still be matrices of other subspaces. Therefore we have
\begin{align*}
G &= \begin{pmatrix} G^{p} & F \\ F & G^{h} \end{pmatrix}, \\
G_{0}^{-1} &= \begin{pmatrix} (G_{0}^{p})^{-1} & 0 \\ 0 & (G_{0}^{h})^{-1} \end{pmatrix}, \tag{16}
\end{align*}
\begin{align*}
\Sigma &= \begin{pmatrix} \Sigma^{p} & S \\ S & \Sigma^{h} \end{pmatrix}.
\end{align*}
We temporarily switch to the bonding-/antibonding ($+, -$) basis
\begin{align*}
2G^{+} &= G^{p} + G^{h}, \\
2G^{-} &= G^{p} - G^{h} \tag{17}
\end{align*}
and for $\Sigma$ and $G_{0}$ accordingly. We expand the correlation functions in Pauli matrices:
\begin{align*}
G &= G^{+} \mathbb{1} + (F, 0, G^{-}) \sigma, \\
\Sigma &= \Sigma^{+} \mathbb{1} + (S, 0, \Sigma^{-}) \sigma, \tag{18}
\end{align*}
The Dyson equation then reads
\begin{align*}
G^{-1} &= (G_{0}^{+} - \Sigma^{+}) \mathbb{1} + (S, 0, G_{0}^{-} - \Sigma^{-}) \sigma. \tag{19}
\end{align*}
The identity
\begin{align*}
GG^{-1} &= 1 \tag{20}
\end{align*}
leads to a set of four equations:
\begin{align*}
1 &= G^{+} \left( G_{0}^{+} - \Sigma^{+} \right) - FS + G^{-} \left( G_{0}^{-} - \Sigma^{-} \right), \tag{21}
0 &= F \left( G_{0}^{+} - \Sigma^{+} \right) - G^{+} S, \tag{22}
0 &= F \left( G_{0}^{-} - \Sigma^{-} \right) + G^{-} S, \tag{23}
0 &= G^{+} \left( G_{0}^{-} - \Sigma^{-} \right) + G^{-} \left( G_{0}^{+} - \Sigma^{+} \right). \tag{24}
\end{align*}
From Eq. (22) and Eq. (23) directly follows
\[
(G^+ - \Sigma^+) = F^{-1}G^+ S, \quad (25)
\]
\[
(G^- - \Sigma^-) = -F^{-1}G^- S, \quad (26)
\]
which we insert in Eq. (21) also backtransforming the
\((+, -)\) basis,
\[
1 = -FS + \frac{1}{2} (G^+ F^{-1} G^h S + G^h F^{-1} G^p S). \quad (27)
\]
With Eq. (28) the first term immediately reads
\[
G^p S G^h S = (G^h F^{-1} - F(G^p)^{-1})^{-1} (G^p F^{-1} - F(G^h)^{-1})^{-1}. \quad (30)
\]
The second involves a bit more algebra:
\[
FS (1 + FS) = (G^p F^{-1} G^h F^{-1} - 1)^{-1} \left( 1 + (G^p F^{-1} G^h F^{-1} - 1)^{-1} \right)
\]
\[
= (G^p F^{-1} G^h F^{-1} - 1)^{-1} G^p F^{-1} G^h F^{-1} (G^p F^{-1} G^h F^{-1} - 1)^{-1}
\]
\[
= (G^h F^{-1} - F(G^p)^{-1})^{-1} (G^p F^{-1} - F(G^h)^{-1})^{-1}. \quad (31)
\]
Furthermore we insert Eq. (22) and Eq. (23) in Eq. (24),
that results in
\[
G^p F^{-1} G^h = G^h F^{-1} G^p. \quad (28)
\]
Finally combining Eq. (27), Eq. (28) gives an expression
for the anomalous part of the self-energy
\[
S = (G^p F^{-1} G^h - F)^{-1} \quad (29)
\]
We substitute it into the coefficient of the local pertur-
bations \(\sim \delta \theta_i^2\) of Eq. (12) and analyse it in two contributions.

III. THERMODYNAMIC LIMIT

We take the thermodynamic limit of the Josephson
lattice model in order to obtain a relation to the macro-
scopic observable, the superconducting stiffness \(I\). Start-
ing from the long-wavelength approximation
\[
H = \frac{1}{2} \sum_{ij} J_{ij} \theta_{ij}^2 \quad (33)
\]
we assume a rather uniform spatial profile of the low-
energy modes. Therefore it is reasonable to interpolate
linearly between the plaquettes \((i, j)\) as we move the them
infinitesimally close together and take the continuum-
limit
\[
\theta_{ij} \to \nabla \theta(r) (r - r') \quad \sum_a \frac{\partial \theta}{\partial r_a} (r - r')_a. \quad (34)
\]
In this limit the Hamiltonian reads
\[
H = \frac{1}{2} \sum_{ab} \int d^4 r \frac{\partial \theta}{\partial r_a} \frac{\partial \theta}{\partial r_b} I_{ab}(r) \quad (35)
\]
with the \(d\)-dimensional unit-cell volume \(V\) and the superconducting stiffness
\[
I_{ab}(r) = \frac{1}{V^2} \int d^4 r' J(r - r') (r - r')_a (r - r')_b. \quad (36)
\]
We substitute \(R = r - r'\) and insert the Fourier repre-
sentation of \(J\):
\[
I_{ab} = \frac{1}{V} \int \frac{d^d q}{(2\pi)^d} \int d^d R e^{iqR} R_a R_b J(q)
\]
\[
= -\frac{1}{V} \partial_{q_a} \partial_{q_b} J(q) \bigg|_{q=0} \quad (37)
\]
with
\[
J(q) = \frac{VT}{(2\pi)^d} \int d^d k \Tr_{\omega_n} \left( F_k S F_{k-q} S - G^p_{k} S G^h_{k-q} S \right) \quad (38)
\]
and thereby show, that the superconducting stiffness \(I_{ab}\)
doesn’t depend on \(r\). Next we have to evaluate the deriva-
tive. After performing the derivative with respect to \(q\),
we can substitute \(k' = k - q\) and perform a partial inte-
gration that leads to
\[
\partial_{q_a} \partial_{q_b} J(q) = -\frac{VT}{(2\pi)^d} \int d^d k' \Tr_{\omega_n} \left\{ \right.
\]
\[
\left. \left( \partial_{k'_a} F_{k'-q} S \left( \partial_{k'_b} F_{k'} S \right) - \left( \partial_{k'_a} G^h_{k'} S \right) \left( \partial_{k'_b} G^p_{k'-q} S \right) \right) \right\} \quad (39)
\]
and in Eq. (37) finally to

\[ I_{ab} = \frac{T}{(2\pi)^d} \int d^d k \text{Tr}_{\omega n} \]

\[ \times (\frac{\partial F(k)}{\partial k_a} S \frac{\partial F(k)}{\partial k_b} S - \frac{\partial G^{\pi}(k)}{\partial k_a} S \frac{\partial G^{\perp}(k)}{\partial k_b} S). \]

Note, that the physical units of the dSC stiffness are restored by

\[ I_{\parallel} \rightarrow \frac{a_a}{a_{\parallel} a_{\parallel}} I_{\parallel}, \quad I_{\perp} \rightarrow \frac{a_c}{a_a a_b} I_{\perp}. \]

In particular for numerical purposes we express the derivatives in terms of derivatives applied to inverse Green functions

\[ \partial_{k_a} G = -G (\partial_{k_a} G^{-1}) G \]

since it reduces the differentiation to that of the electron dispersion \( G^{-1}(k) \sim t(k) \). Regarding the number of \( k \)-points per dimension and Matsubara frequencies \( \omega_n \) we choose \( N_k = N_{\omega_n} = 64 \) which is sufficient for an accuracy of \( \sim 10^{-7} \), see Fig. 2 and Fig. 3.

FIG. 2. Convergence of the dSC stiffness \( I \) with number of Matsubara frequencies \( \omega_n \) \( (N_{\omega_n}^{max} = N_k = 128) \).

FIG. 3. Convergence of the dSC stiffness \( I \) with number of \( k \)-points per dimension \( (N_k^{max} = N_{\omega_n} = 128) \).

IV. CDMFT

We solve the CDMFT\[4-6\] equation

\[ G^{-1}(i\omega_n) = \left( \sum_k G(i\omega_n, k) \right)^{-1} + \Sigma(i\omega_n), \]

\[ G^{-1}(i\omega_n, k) = i\omega_n + \mu - t(k) + \Sigma(i\omega_n) \]

with the lattice dispersion of the reduced Brillouin zone \( t(k) \) numerically\[7, 8\] and obtain the self-consistent local lattice Green function that is the first term of Eq. (43). CDMFT maps the lattice problem to a multi-orbital Anderson impurity model, in that the different orbitals also represent the sites of the cluster. The Anderson impurity model of arbitrary local interactions can be solved exactly by the use of the continuous-time quantum Monte-Carlo method (CTHYB). The bath of that model is dynamical and so is the mean-field of CDMFT. But the temporal correlations exist only locally, i.e., on the cluster. Therefore the self-energy between clusters vanishes.

Using the symmetry of the plaquette, the local Green function has the blockstructure

\[ G_{loc} = \begin{pmatrix} G_T & G_X \\ G_Y & G_M \end{pmatrix} \]

where we labeled the plaquette orbitals according to the same transformation properties of the high-symmetry points of the Brillouin zone of the square lattice. The transformation from site-space to plaquette orbitals is a unitary transformation with

\[ U = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & -1 & 1 \end{pmatrix} \]

In principle antiferromagnetic order can also be considered, but it would reduce the blockstructure of Eq. (45) and will be computationally more expensive.

In our CDMFT approximation the self-energy exists only within the cluster and not between clusters. In order to obtain the lattice Green function one could try to interpolate the many-body correlations between the clusters. This procedure is ambiguous. Following the idea of supersites we do not interpolate the self-energy. Therefore the lattice Green function reads

\[ G(i\omega_n, r) = \frac{1}{N_k} \sum_k e^{ikr} \]

where \( r \) are cluster-translations and \( i\omega_n, \mu, t(k) \) and \( \Sigma(i\omega_n) \) are matrices in Nambu plaquette-orbital or site-basis. \( k \) is in the reduced Brillouin zone according to plaquette translations. For the CDMFT calculations we use 1025 Matsubara frequencies, 64 \( k \)-points per dimension, \( 192 \times 10^5 \) Monte-Carlo (MC) measurements, 200
updates per MC measurement and $3 \times 10^3$ MC warm-up cycles. The number of Legendre-coefficients for the representation of the Green function, that we measure in the Monte-Carlo process, depends mostly on the temperature. A reasonable range for our calculations is 50-150. During the CDMFT loops we perform partial updates of the self-energy using a mixing parameter of 0.5. For the dSC symmetry breaking we initialized the CDMFT cycles with a symmetry broken self-energy.

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