




Collective magnetic fluctuations in Hubbard plaquettes captured by fluctuating local field methodAlexey N. Rubtsov ^{1,2,*}, Evgeny A. Stepanov ^{3,4} and Alexander I. Lichtenstein ^{3,5,4}¹*Russian Quantum Center, Skolkovo Innovation City, 121205 Moscow, Russia*²*Department of Physics, Lomonosov Moscow State University, Leninskie Gory 1, 119991 Moscow, Russia*³*I. Institute of Theoretical Physics, Department of Physics, University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany*⁴*Theoretical Physics and Applied Mathematics Department, Ural Federal University, Mira Street 19, 620002 Ekaterinburg, Russia*⁵*European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany*

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We establish a way to handle main collective fluctuations in correlated quantum systems based on a fluctuating local field concept. This technique goes beyond standard mean-field approaches, such as Hartree-Fock and dynamical mean-field theories (DMFT), as it includes a fluctuating classical field that acts on the leading order parameter of the system. Effective model parameters of this theory are determined from the variational principle, which allows one to resolve the Fierz ambiguity in decoupling of the local interaction term. In the saddle-point approximation for the fluctuating field our method reproduces the mean-field result. The exact numerical integration over this field allows one to consider nonlinear fluctuations of the global order parameter of the system while local correlations can be accounted for by solving the DMFT impurity problem. We apply our method to the magnetic susceptibility of finite Hubbard systems at half-filling and demonstrate that the introduced technique leads to a superior improvement of results with respect to parental mean-field approaches, without significant numerical complications. We show that the fluctuating local field method can be used in a very broad range of temperatures substantially below the Néel temperature of DMFT, which remains a major challenge for all existing theoretical approaches.

DOI: [10.1103/PhysRevB.102.224423](https://doi.org/10.1103/PhysRevB.102.224423)**I. INTRODUCTION**

The theoretical description of collective effects of interacting fermionic systems is one of the main problems of modern physics. In correlated materials, these collective electronic fluctuations form effective bosonic modes, such as plasmons, magnons, etc., that may possess a nonlinear behavior. The origin of such behavior can be both the interaction between different modes as well as the anharmonic fluctuation of the single mode itself. At low temperatures, the presence of these instability channels may result in a spontaneous symmetry breaking associated with the formation of ordered phases in the system. Strong collective fluctuations appear not only in infinite crystal lattices, but also in other physical systems that are not necessarily large and can be essentially finite. In this regard, we mention vibrational modes in nuclei [1], breathing modes [2] and short-range charge and spin correlations [3–6] in systems of ultracold atoms trapped in optical lattices, and collective spin modes in molecular magnets [7–9].

A large collection of theoretical approaches from simple mean-field theories [10–13] and rotationally invariant path-integral schemes [14–21] to much more advanced methods [22] has been developed in order to describe these collective effects. The simplest mean-field theory, namely the Hartree-Fock (HF) method [23,24], is able to capture a spontaneous symmetry breaking in weakly interacting systems.

For strong correlations, the preference is often given to a polarized dynamical mean-field theory (DMFT) [25]. This approach relies on the exact numerical solution of an effective impurity problem, which provides an accurate approximation for local observers [26]. Various diagrammatic extensions of DMFT have been constructed to handle nonlocal correlations underlying the formation of collective electron modes [22]. A particular subset of diagrams varies for different methods, and may contain either simple *GW*-like diagrams [27–33] including vertex corrections [34–37], or more complex ladder [38–45] and parquet [46] contributions, as well as all possible diagrammatic terms up to a certain order of perturbation expansion [47–49].

Diagrammatic techniques introduced on top of DMFT are currently seen as the most advanced and promising tools for description of collective fluctuations in correlated systems. It should be mentioned, however, that applicability of these computational scheme is limited, because it implicitly exploits an assumption of a weak anharmonicity of collective modes. Indeed, collective nonlocal effects in these approaches are considered perturbatively, so that only (nearly) harmonic fluctuations of the corresponding order parameter are taken into account. This assumption works reasonably well at high temperatures and/or in high dimensions [44,50–53]. However, strong collective fluctuations that are supposed to break the ordering at low temperatures are strongly nonlinear. It can be expected that such physics is particularly important for antiferromagnetic (AFM) fluctuations, since the AFM order parameter obeys strong quantum zero-point fluctuations even

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for three-dimensional (3D) bulk materials, whereas in 2D the ordering at finite temperatures is forbidden by the Mermin-Wagner theorem [54]. We also believe that the nonlinearity of collective fluctuations is a fundamental reason why all the introduced above diagrammatic extensions of DMFT, as well as exact diagrammatic Monte Carlo approaches [55–60], do not allow for a quantitative description of the 2D Hubbard model substantially below the DMFT Néel point [61]. In this regard, the desired improvement of the theory for strong collective fluctuations especially at low temperatures calls for new ideas.

In this work we turn off the beaten path of doing a perturbative expansion around the mean-field result, and present a method that is capable of describing nonlinear collective fluctuations in finite systems at low temperatures. For the sake of concreteness, we apply the formulated theory to small Hubbard plaquettes. Among all mentioned systems that possess strong collective fluctuations, the considered model is mostly close to molecular magnets. However, we would like to point out that the present scheme is rather general and can be constructed for any system where developed collective fluctuations belong to the one or several leading collective modes. In addition, the result for small Hubbard lattices at half-filling can also be efficiently benchmarked, because quantum Monte Carlo (QMC) simulations for such lattices do not suffer from the sign problem [62] and therefore can provide reliable reference data.

We note that the correct description of the AFM susceptibility of these small systems, which we aim to address in this paper, is already a challenging problem. For example, our calculations show that for a 4×4 square plaquette with periodic boundary conditions applicability of the best local mean-field approximation, namely DMFT, is limited to a temperature of about $U/8$, where U is the on-site Coulomb potential. At a twice smaller temperature, this approach that neglects nonlocal correlations shows an unphysical Néel transition. At the same time, a spatial pattern of AFM fluctuations on finite plaquettes is expected to be rather simple. In this case, the small number of lattice sites results in a coarse grid for the Brillouin zone. Then, already a single AFM mode, which is associated with the $Q = \{\pi, \pi\}$ momentum, should capture the most important physics of spin fluctuations in the system. Fluctuations with other wave vectors in small systems are not important, because the AFM correlation length is larger than the system size.

Consequently, one can introduce a Landau free energy $\mathcal{F}(m)$, where magnetization of the AFM sublattices m serves as a “global” order parameter. According to Landau phenomenology, at low temperatures the second derivative of the free energy $\partial_m^2 \mathcal{F}(m)|_{m=0}$ becomes negative, and $\mathcal{F}(m)$ takes the form of a Mexican hat potential (see Fig. 1). As mentioned above, diagrammatic schemes built on top of DMFT partly take collective electronic effects into account, introducing a renormalization for a corresponding two-particle fluctuation. However, consideration of a leading subset of diagrams implies that a small nonlinearity of fluctuations is assumed. Taking strong nonlinearity into account formally requires to sum over all diagrams, as done, for example, in diagrammatic QMC calculations [55–60]. Note is that this exact perturbation expansion does not converge at low temper-

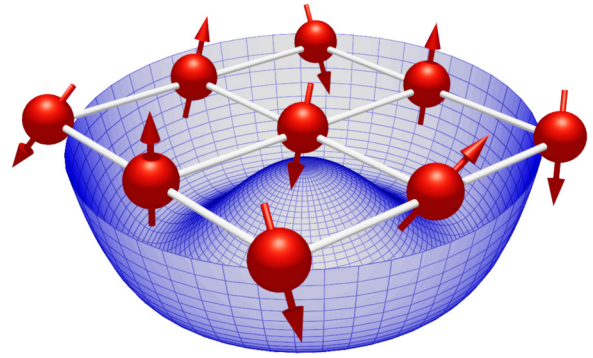


FIG. 1. Sketch of spin fluctuations (red arrows) in a Hubbard plaquette near the antiferromagnetic state, which is described by an effective Mexican hat potential (blue).

atures, and a renormalization procedure is required to achieve physically interesting regimes [63]. Thus we conclude that diagrammatic schemes on the basis of DMFT are justified until a Mexican hat potential is formed [61]. At the same time, their applicability at lower temperatures, where fluctuations of the order parameter become essentially unharmonic, is questionable. In addition, we find diagrammatic extensions of DMFT technically too complicated for the rather simple system under investigation. Instead, here we propose a solution of the problem introducing an effective local field that mediates nonlinear fluctuations of the order parameter we are interested in. To this aim we build a fluctuating local field (FLF) approach on the basis of two mean-field schemes starting from Hartree-Fock and DMFT solutions of the problem. Previously, a similar approach was invented for classical lattices [64]. The introduced FLF method is numerically inexpensive and does not bring a sufficient complication to its parental mean-field theory. In particular, the FLF scheme built on top of DMFT does not involve any calculation of two-particle vertices of the impurity problem, or similar quantities. At the same time, nonlinear collective AFM fluctuations are explicitly included in this scheme and accounted exactly. Thus, the theory unperturbatively accounts for both local correlations and collective fluctuations by solving the DMFT impurity problem and integrating over the fluctuating field. We compare our results to the QMC reference data for 4×4 , 6×6 , and 8×8 square plaquettes, and demonstrate that the introduced FLF technique leads to an impressive improvement of mean-field results.

II. THEORY

A. Definitions

Our goal is to address spin fluctuations of small correlated lattices. Whereas the following consideration can be applied to quite wide class of systems, we stick to a particular case of a half-filled Hubbard model on a square lattice with the following action:

$$\mathcal{S}[c^\dagger, c] = -c_1^\dagger \mathcal{G}_{12}^{-1} c_2 + U(n_{j\tau\uparrow} - \frac{1}{2})(n_{j\tau\downarrow} - \frac{1}{2}). \quad (1)$$

Here, $c^{(\dagger)}$ are Grassmann variables corresponding to the annihilation (creation) of electrons. Subscripts “1” and “2” are combined indices of the lattice site j (or momentum \mathbf{k}), imaginary time τ (or Matsubara frequency $\omega = \pi(2p+1)/\beta$,

$p \in \mathbb{Z}$), and spin projection $\sigma = \{\uparrow, \downarrow\}$. $n_{j\tau\sigma} = c_{j\tau\sigma}^\dagger c_{j\tau\sigma}$ describes the electron density and β is the inverse temperature. Throughout the paper, tensor notation is used, so that the summation is taken over repeated indices. The bare Green's function reads

$$\mathcal{G}^{-1} = i\omega - \varepsilon + h^l \Lambda_Q^l, \quad (2)$$

where the dispersion $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ is the Fourier transform of the nearest-neighbor hopping amplitude t . Note that here we additionally account for an external AFM field \mathbf{h} . The tensor Λ_Q describes the coupling of the field \mathbf{h} to fermion degrees of freedom. Its explicit structure can be seen from the following expression:

$$c_1^\dagger \mathcal{G}_{12}^{-1} c_2 = c_{\mathbf{k}\omega\sigma}^\dagger (i\omega - \varepsilon_{\mathbf{k}}) c_{\mathbf{k}\omega\sigma} + c_{\mathbf{k}\omega\sigma}^\dagger \sigma_\sigma^l h^l c_{\mathbf{k}+Q,\omega,\sigma'}, \quad (3)$$

where $Q = \{\pi, \pi\}$ is the AFM wave vector and σ^l is the $l = \{x, y, z\}$ component of the vector of Pauli matrices. The field \mathbf{h} is then coupled to the AFM-ordered variable $M_Q^l = c_1^\dagger \Lambda_{12}^l c_2$ that describes polarization of electrons. Then, the average $\mathbf{m} = \frac{1}{\beta N} \langle \mathbf{M} \rangle$ is the AFM order parameter of the system. While constructing the formalism, it is convenient to keep \mathbf{h} finite. A paramagnetic solution can be obtained taking the limit $\mathbf{h} \rightarrow 0$ afterwards.

B. Resolution of Fierz ambiguity

The goal of the FLF approach is to identify the leading instability in the system, which is to be accounted for exactly, neglecting other less important modes. The procedure has to be performed carefully, because it may lead to hidden problems such as Fierz ambiguity [65–67]. To illustrate this point, let us consider the initial problem (1) in a mean-field approximation. For this aim we rewrite the on-site Coulomb potential in terms of spin densities as

$$U(n_{j\tau\uparrow} - \frac{1}{2})(n_{j\tau\downarrow} - \frac{1}{2}) = -\frac{1}{2} s_{j\tau}^l \mathcal{U}_{ll'} s_{j\tau}^{l'}, \quad (4)$$

where $s^l = c_\sigma^\dagger \sigma_\sigma^l c_\sigma$ is the l projection of the spin density, and \mathcal{U} is an arbitrary symmetric 3×3 matrix with the constrained trace $\text{Tr} \mathcal{U} = U$. In what follows we assume for simplicity that \mathcal{U} has an inverse. In special cases when this is not the true, one can consider some approximation or a particular block of \mathcal{U} that is invertible. This decoupling of the local Coulomb interaction can also be done with inclusion of charge degrees of freedom. However, the latter are not of the interest for the current work, because they do not represent the main instability of the considered system.

The mean-field description of spin degrees of freedom can be performed introducing an effective vector field φ via Hubbard-Stratonovich transformation of the interaction term (4). The partition function of the problem can now be rewritten as $\mathcal{Z} = \int D[\varphi] D[c^\dagger, c] e^{-S[c^\dagger, c, \varphi]}$, where

$$S[c^\dagger, c, \varphi] = -c_1^\dagger \mathcal{G}_{12}^{-1} c_2 - \varphi_{j\tau}^l s_{j\tau}^l + \frac{1}{2} \varphi_{j\tau}^l \mathcal{U}_{ll'}^{-1} \varphi_{j\tau}^{l'}. \quad (5)$$

The mean-field value φ_{MF} can be obtained from the saddle-point approximation for the integral over the vector field φ , which can be expressed in the following condition:

$$\delta S[\varphi_{\text{MF}}] = 0. \quad (6)$$

Here, the action for Hubbard-Stratonovich fields

$$S[\varphi] = -\ln \det [\mathcal{G}^{-1} + \varphi^l \Lambda_Q^l] + \frac{1}{2} \varphi_{\tau j}^l \mathcal{U}_{ll'}^{-1} \varphi_{\tau j}^{l'} \quad (7)$$

can be obtained after integrating out fermion degrees of freedom in Eq. (5) leading to $\mathcal{Z} = \int D[\varphi] e^{-S[\varphi]}$. This results in $\varphi_{\text{MF}}^l = \frac{1}{2} \mathcal{U}_{ll'} \langle s^{l'} \rangle$, and we get a mean-field approximation for the action (5),

$$\mathcal{S}_{\text{MF}}[c^\dagger, c] = -c_1^\dagger \mathcal{G}_{12}^{-1} c_2 - \varphi_{\text{MF}}^l M_Q^l, \quad (8)$$

that describes noninteracting fermions in the presence of an effective field:

$$h_{\text{eff}}^l = h^l + \frac{1}{2} \mathcal{U}_{ll'} m_{\text{MF}}^{l'}. \quad (9)$$

Here, \mathbf{m}_{MF} is the average AFM magnetization of the mean-field problem (8). Now, it becomes clear that the obtained result crucially depends on a particular choice of the matrix \mathcal{U} leading to Fierz ambiguity in decoupling of the interaction term. Indeed, considering the spin polarization along the z axis, we get $\varphi_{sp}^z = \frac{1}{2} \mathcal{U}_{zz} m^z$, where \mathcal{U}_{zz} in the isotropic decoupling form $\mathcal{U}_{xx} = \mathcal{U}_{yy} = \mathcal{U}_{zz} = U/3$ is three times smaller than in the Ising form, where only the z component of the spin is considered: $\mathcal{U}_{zz} = U, \mathcal{U}_{xx} = \mathcal{U}_{yy} = 0$.

Remarkably, not only simple mean-field theories suffer from the Fierz ambiguity. This issue is also present in more elaborate methods like the GW +EDMFT approach [27–33] and the triply irreducible local expansion (TRILEX) [34–36] that have been introduced to solve strongly interacting electronic problems. A physical reason for Fierz ambiguity is that Hubbard-Stratonovich fields φ exhibit strong fluctuations, which make the saddle-point approximation for the integral inaccurate. All theories that treat the interaction in a mean-field form effectively perform an expansion around the saddle-point approximation. Different decouplings of the on-site Coulomb potential (4) produce different fluctuation patterns and different mean-field solutions for the same initial problem, and it is not *a priori* clear which form of the interaction should be chosen. In principle, the Fierz ambiguity can be avoided if the interaction is taken in the form that provides the most accurate result for some quantity that can be calculated exactly. Recently, this idea has been exploited for the derivation of the interaction for the DMFT-based dual TRILEX (D-TRILEX) method, by approximating the exact renormalized local fermion-fermion interaction [37]. Importantly, it was argued that the most accurate form of the effective interaction $\mathcal{U}_{ll'}$ cannot be obtained by any decoupling of the on-site Coulomb potential. Here, we show that the Fierz ambiguity can also be cured by a renormalization of parameters of an effective theory.

Let us consider the problem (8) as a trial action, where an effective field φ_{eff} plays a role of a free parameter that may differ from the saddle-point value φ_{MF} . This parameter can be chosen, for example, using the Peierls-Feynman-Bogoliubov variational principle [68–70] for the functional

$$\mathcal{F}(\varphi_{\text{eff}}) = \mathcal{F}_{\text{MF}}(\varphi_{\text{eff}}) + (\beta N)^{-1} \langle S[c^\dagger, c] - \mathcal{S}_{\text{MF}}[c^\dagger, c] \rangle_{\text{MF}}. \quad (10)$$

Here, $S[c^\dagger, c]$ is the initial action (1), $\mathcal{F}_{\text{MF}}(\varphi_{\text{eff}})$ is the free energy of the mean-field action (8), and $\langle \dots \rangle_{\text{MF}}$ denotes averaging with respect to the mean-field partition function \mathcal{Z}_{MF} .

An optimal value of φ_{eff} can be found minimizing the energy $\partial_{\varphi_{\text{eff}}}\mathcal{F}(\varphi_{\text{eff}}) = 0$. This consideration gives a well-known Hartree-Fock result

$$h_{\text{eff}}^l = h^l + \frac{1}{2}U m_{\text{MF}}^l \quad (11)$$

that does not depend on the form of the decoupling (4). Importantly, this variational solution of the problem is not only unambiguous, but also known to provide a quantitatively correct result at least for weakly correlated systems in high dimensions.

The above consideration may look rather trivial, but it serves as a very instructive starting point for construction of the fluctuation local field method. Indeed, the optimal value of the effective field φ_{eff} obtained via the Peierls-Feynman-Bogoliubov variational principle does not depend on the decoupling. This means that the same result (11) can also be obtained in the saddle-point approximation (9), but only for one particular decoupling (4), which in our case corresponds to the Ising form discussed above. The saddle-point approximation of an integral is convenient from many points of view. Therefore, instead of finding a particular decoupling form of the on-site Coulomb potential (4), we propose to consider the following renormalization procedure that improves the saddle-point approximation. From a mathematical point of view, this can be performed taking into account a matrix of second derivatives (curvature) of the field φ at the φ_{MF} point. Formally this means that the action that enters the extremum condition (6) should be changed to $\mathcal{S}[\varphi] + \mathcal{S}'[\varphi]$. Instead of the explicit calculation of $\mathcal{S}'[\varphi]$, we assume that it can be accounted for by a proper renormalization of the “stiffness” \mathcal{U}^{-1} in Eq. (7) calculated at the saddle point. Practically, we adjust \mathcal{U} to get a saddle-point approximation (6) coinciding with the HF result (11). For example, for the isotropic decoupling this condition gives $\mathcal{U}_{xx} = \mathcal{U}_{yy} = \mathcal{U}_{zz} = U$. We note that such a renormalized interaction \mathcal{U}_{ij} is not trace constrained anymore and thus cannot be obtained by decoupling the local Coulomb interaction (4). In this sense, the presented idea is consistent with the result of the D-TRILEX method [37]. The use of the renormalized low-energy interaction for Hubbard-Stratonovich fields is one of the key ingredients of the FLF approach presented below.

C. FLF on top of Hartree-Fock method

There are two assumptions underlying the HF theory. First, the interaction U should be small enough to neglect higher-order corrections to an effective field (11). Second, even a weakly interacting system can exhibit strong collective fluctuations that are neglected in the HF scheme. Thus, an improvement of the HF theory would naturally require one to account for these collective fluctuations. Following the pathway proposed in Ref. [64] this can be done replacing the constant effective HF field φ_{eff} (11) by a fluctuating vector field V , introducing an *ensemble* of effective Gaussian actions

$$\mathcal{S}_{\text{FLF}}[c^\dagger, c, V] = -c_1^\dagger \mathcal{G}_{12}^{-1} c_2 - V^l M_Q^l + \frac{1}{2} \frac{\beta N}{J_Q} \mathbf{V}^2. \quad (12)$$

Importantly, this action is different from the exact one (5) that represents the initial theory. Here, unlike quantum Hubbard-Stratonovich fields $\varphi_{j\tau}$, we deal with a classical

three-component vector field V that describes only the leading magnetic mode with the zero bosonic frequency $\Omega = 0$ and AFM momentum $Q = (\pi, \pi)$. Other fluctuations, as well as quantum fluctuations of the isolated AFM mode, are neglected, since the field V does not depend on j and τ . One can expect that our approach is particularly relevant for small lattices, where only one discrete \mathbf{q} -mode softens and becomes essentially unharmonic at low temperatures. However, the role of quantum fluctuations described by $\Omega \neq 0$ is *a priori* not clear and will be addressed further. It is important that no assumption is made about the magnitude of AFM fluctuations or whether they are harmonic or not.

We have shown previously that simply neglecting fluctuations in high-energy modes may lead to incorrect results. Following the receipt obtained in Sec. II B, this issue is solved by introducing a renormalization of the interaction via a “stiffness” parameter J_Q . The former can be chosen in different and, generally speaking, nonequivalent ways. First, let us assume for a moment that the integral over V in the partition function

$$\mathcal{Z}_{\text{FLF}} = \int D[c^\dagger, c] d^3V e^{-\mathcal{S}_{\text{FLF}}[c^\dagger, c, V]} = \int d^3V e^{-\mathcal{S}_{\text{FLF}}[V]} \quad (13)$$

is estimated from the saddle-point approximation (6), where

$$\mathcal{S}_{\text{FLF}}[V] = -\ln \det [\mathcal{G}^{-1} + V^l \Lambda_Q^l] + \frac{1}{2} \frac{\beta N}{J_Q} \mathbf{V}^2. \quad (14)$$

Straightforwardly, one gets

$$V_{\text{MF}}^l = J_Q m^l. \quad (15)$$

Physically, the saddle-point approximation means that fluctuations of the field V are neglected. It is worth mentioning that the average magnetization m^l contains an effect of an external field h via the bare Green’s function (2). Noting that V_{MF} also acts as a polarized AFM field, it is reasonable to demand that for any value of the external field h the saddle point approximation should reproduce the HF result (11), which also does not account for fluctuations of the order parameter. This immediately results in the $J_Q = U/2$ value of a stiffness constant. Now, when all parameters of the FLF action (12) are identified, the integral over the field V can be taken numerically exactly after integrating out fermion degrees of freedom.

It is worth noting that the self-consistent Hartree-Fock result (11) and, consequently, V_{MF} change dramatically upon lowering the temperature. Whereas at high temperatures an effective field h_{eff} is proportional to the external field h , below the HF Néel point the average magnetization m is finite even for an infinitesimal h . Nevertheless, our saddle-point analysis results in the same constant value $J_Q = U/2$ within the entire temperature range.

There exists another possibility of how the stiffness parameter J_Q can be chosen. Instead of finding the value of J_Q that reproduces the Hartree-Fock result (11), which is obtained via the Peierls-Feynman-Bogoliubov variational principle (10), one can directly use J_Q as a variational parameter for the mapping of the original model (1) onto a trial action (12). For this aim, the FLF V in Eq. (12) can be integrated out directly,

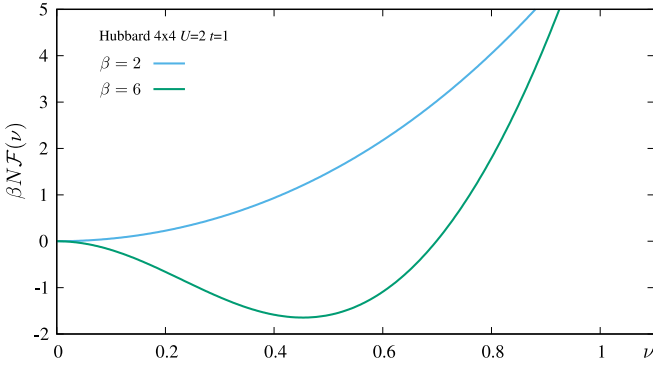


FIG. 2. The value of $\beta N \mathcal{F}(V)$ for the FLF-HF theory plotted as a function of the field V . Upper (blue) and lower (green) curves are obtained for regions below ($\beta = 2$) and above ($\beta = 6$) the HF Néel point $\beta_N \approx 3.8$, respectively.

which results in the following trial action:

$$\mathcal{S}_{\text{FLF}}^*[c^\dagger, c] = -c_1^\dagger G_{12}^{-1} c_2 - \frac{1}{2} \frac{J_Q}{\beta N} M_Q' M_Q'. \quad (16)$$

Using the same variational principle for the functional (10), where the mean-field action $\mathcal{S}_{\text{MF}}[c^\dagger, c]$ is now replaced by the trial action $\mathcal{S}_{\text{FLF}}^*[c^\dagger, c]$, one analytically gets $J_Q \simeq U/2$. In addition, we also performed a direct numerical minimization of the functional, which gave $J_Q \simeq U/2$ as well. A detailed derivation of this result can be found in the Supplemental Material (SM) [71].

To get further insight into the method and obtain an additional justification of our choice of J_Q , it is instructive to see how the Landau free energy $\mathcal{F}(V) = (\beta N)^{-1} \mathcal{S}(V)$ behaves at $h = 0$. The value of $\mathcal{F}'(V) = -(\beta N)^{-1} \ln \det [\mathcal{G}^{-1} + V^l \Lambda_Q^l]^{-1}$ decreases with an increase of V . For small V , the system responds linearly, so that $\mathcal{F}'(V \rightarrow 0) = \mathcal{F}'(0) - \frac{1}{2} \chi_0 V^2$, where χ_0 is the bare static susceptibility of the lattice. Therefore, $\mathcal{F}(V)$ exhibits a minimum (maximum) at $V = 0$ if χ_0 is smaller (larger) than J_Q^{-1} . It can be shown that for $J_Q = U/2$ the transition between two regimes occurs at the HF Néel temperature. For large V , the spin polarization saturates at some m_{max} , so that $\mathcal{F}'(V \rightarrow \infty) = -V m_{\text{max}}$. Therefore, the term $\frac{1}{2} J_Q^{-1} V^2$ dominates at large V , which guarantees a convergence of the integral in \mathcal{Z}_{FLF} . This qualitative behavior of $\mathcal{F}(V)$ resembles what one would expect for the Landau free energy of a phenomenological theory for a critical phenomenon. However, there are important differences. First, in our consideration $\mathcal{F}(V)$ is not a function of the order parameter m but of an effective field V that acts on the order parameter. Second, $\mathcal{F}(V)$ is different from the common 2-4 form of the double-well potential. In particular, it shows $\propto V^2$ behavior at large V .

Now let us discuss the role of fluctuations using a specific example. Figure 2 shows behavior of the Landau free energy for the 4×4 plaquette for $U = 2t$. We plot $\beta N \mathcal{F}(V)$ for two inverse temperatures $\beta = 6$ and $\beta = 2$ below and above the HF transition point, respectively. For high temperature the curve shows a single minimum at $V = 0$. Below the HF transition point the system reveals phase (Goldstone) fluctuations originating from a degeneracy of the minimum of the Mexican hat potential. The amplitude of fluctuations can be estimated

from regions where $\beta N \mathcal{F}(V)$ deviates from its minimal value by ~ 1 . This deviation corresponds to an exponential change of the energy defined by the partition function \mathcal{Z} . As one can see, these regions are remarkably broad, although both values $\beta = 2$ and $\beta = 6$ are not very close to the HF Néel point $\beta \approx 3.8$. Thus, it can be concluded that small Hubbard lattices indeed exhibit strong non-Gaussian fluctuations of the order parameter within a broad temperature interval.

D. FLF on top of the DMFT approach

For U larger than several hopping amplitudes t , the Hubbard model exhibits strong correlations. They are manifested in a local moment formation and appearance of Hubbard subbands in a single-particle spectrum. This physics is not captured by the Hartree-Fock method. In this regime dynamical mean-field theory is more suited to address this problem. Within the DMFT, local correlations are taken into account exactly and unperturbatively with the help of an auxiliary local system

$$\mathcal{Z}_{\text{imp}}^{(j)}[c^\dagger, c] = -c_{j\omega\sigma}^\dagger (i\omega - \Delta_{j\omega}^{\sigma\sigma'}) c_{j\omega\sigma'} + U(n_{j\tau\uparrow} - \frac{1}{2})(n_{j\tau\downarrow} - \frac{1}{2}). \quad (17)$$

Here, the introduced hybridization function Δ is local in space, which allows one to solve this single-site impurity problem exactly and obtain the local Green's function G_{imp} . The DMFT partition function then reads (see Ref. [72], and also SM [71] for a different derivation)

$$\mathcal{Z}_{\text{DMFT}} = \mathcal{Z}_{\text{imp}} \det G_{\text{imp}} \det G_{\text{DMFT}}^{-1} = \mathcal{Z}_{\text{imp}} \det [1 + G_{\text{imp}}(\Delta - \varepsilon + h^l \Lambda_Q^l)], \quad (18)$$

where \mathcal{Z}_{imp} is the partition function of the impurity problem (17), and G_{DMFT} is the DMFT Green's function that can be found from the relation

$$G_{\text{DMFT}}^{-1} = G_{\text{imp}}^{-1} + \Delta - \varepsilon + h^l \Lambda_Q^l. \quad (19)$$

The hybridization function Δ is obtained using the self-consistency condition that the local part of the DMFT Green's function is equal to the impurity Green's function.

The important physics that can be captured by DMFT is primarily related with a formation of a local magnetic moment at each lattice site. Inclusion of the frequency-dependent hybridization function Δ_ω allows one to account for a formation of the local moment, which is important for the Mott physics. However, in the paramagnetic regime local moments at different lattice sites are not correlated, and these collective fluctuations are missing at the DMFT level. To get an inspiration how the DMFT can be improved, it is instructive to consider a finite Hubbard lattice at low temperatures. According to the Mermin-Wagner theorem this system is paramagnetic. Therefore, at $h = 0$ one should formally deal with a nonpolarized DMFT solution associated with a spin-independent hybridization function Δ^0 and Green's function G_{imp}^0 . However, this approximation turns out to be unsatisfactory, because G_{imp}^0 does not contain information about the local magnetic moment of the impurity problem, which exhibits strong fluctuations around its zero average value. Moreover, these fluctuations are characterized by a much

smaller timescale than a single-particle dynamics described by a single-electron Green's function. Thus, it would be physically correct to replace G_{imp}^0 in (19) by an ensemble of polarized Green's functions that provide different realizations of the local spin moment. For this aim we introduce the FLF-DMFT approach described below.

Following the strategy we have used to improve the Hartree-Fock theory, we assume that magnetic fluctuations in the system are represented by a classical AFM vector field V , so that the fluctuating Green's function of the auxiliary system equals $G_{\text{imp}}^0 - V^l L_Q^l$. Here L_Q is a tensor quantity similar to Λ_Q in Eq. (2) that additionally carries an ω frequency dependence. Then, the FLF-DMFT partition function can be written as $\mathcal{Z}_{\text{FLF}} = \mathcal{Z}_{\text{imp}} \int d^3 V e^{-\mathcal{S}_{\text{FLF}}[V]}$ with

$$\mathcal{S}_{\text{FLF}}[V] = -\ln \det \left[1 + (G_{\text{imp}}^0 - V^l L_Q^l) (\Delta^0 - \varepsilon + h^l \Lambda_Q^l) \right] + \frac{1}{2} \frac{\beta N}{J_Q} \mathbf{V}^2 \quad (20)$$

where the FLF-DMFT Green's function is (see SM [71])

$$G_{\text{FLF}} = \left\langle \frac{1}{(G_{\text{imp}}^0 - V^l L_Q^l)^{-1} + \Delta^0 - \varepsilon + h^l \Lambda_Q^l} \right\rangle_{\text{FLF}}. \quad (21)$$

It is important to compare expressions for FLF-HF (14) and FLF-DMFT (20). They are essentially different in the way how the FLF is introduced. In FLF-HF fluctuations are associated with an effective field (9), which is, in fact, the only adjustable parameter of the HF theory. In contrast, as can be seen from Eq. (19), there are *two* quantities that appear in DMFT: hybridization function Δ and Green's function G_{imp} . One could introduce a theory where fluctuations are associated with the hybridization function. In this case, the theory will be similar to the FLF-HF approach, where the saddle-point approximation for the FLF reproduces the polarized local self-energy (see SM [71]). However, a physical picture of a fluctuating local moment suggests a different approach expressed by Eq. (20), where fluctuations of the local Green's function are considered. Nevertheless, in the former case a direct connection between the FLF-HF and FLF-DMFT theories can still be established. As we show in SM [71], this form of the FLF-DMFT approach can be seen as FLF-HF theory introduced for effective fermion variables in a dual space.

The saddle-point estimation for the Green's function (21) is

$$G_{\text{FLF}}^{\text{MF}-1} = (G_0^{\text{imp}} - V_{\text{MF}}^l L_Q^l)^{-1} + \Delta_0 - \varepsilon + h^l \Lambda_Q^l, \quad (22)$$

where V_{MF} can be found from the saddle-point equation

$$J_Q^{-1} \mathbf{V}_{\text{MF}}^2 = \text{Tr} \frac{-V_{\text{MF}}^l L_Q^l}{(\Delta^0 - \varepsilon + h^l \Lambda_Q^l)^{-1} + G_{\text{imp}}^0 - V_{\text{MF}}^l L_Q^l}. \quad (23)$$

In analogy with the previous consideration, we determine $V_{\text{MF}}^l L_Q^l$ from the observation that $G_{\text{FLF}}^{\text{MF}}$ corresponds to a polarized theory, where nonlocal fluctuations are neglected. Therefore, it should coincide with a known mean-field result. Whereas the saddle-point value of the FLF (15) within the FLF-HF scheme was determined from the polarized HF result, here we require that (22) reproduces the polarized DMFT

solution (19). This results in the following relation:

$$V_{\text{MF}}^l L_Q^l = G_{\text{imp}}^0 \bar{\Sigma} G_{\text{imp}}^0, \quad (24)$$

where $\bar{\Sigma}^{-1} = \delta \Sigma_{\text{imp}}^{-1} + G_{\text{imp}}^0$, and $\delta \Sigma_{\text{imp}}$ is the difference between the non-polarized and polarized self-energies of DMFT. This relation defines the frequency-dependent profile of the tensor quantity $L_Q \omega$.

From the very beginning, the FLF V and function L_Q are introduced as a scalar product. This gives us the freedom to choose both quantities separately up to a rescaling parameter. For numerical calculations it is convenient to use the normalized value of the FLF imposing that $\|\mathbf{V}_{\text{MF}}^2\| = 1$. Then, substituting the result of Eq. (24) to Eq. (23), one immediately finds an effective stiffness constant J_Q . Note that, the proposed choice for the saddle-point value of the FLF (24) is not unique. In principle, one can find other physical arguments to fix V_{MF} . One more possibility that determines the saddle point is discussed in SM [71]. However, we find that it does not lead to a noticeable change of the result of the introduced FLF-DMFT theory.

III. NUMERICAL RESULTS

In this section we present numerical results for the Curie constant $C = \beta^{-1} \partial_h \langle s \rangle$ for Hubbard plaquettes with periodic boundary conditions. Two regimes, a moderate ($U = 2t$) and a strongly ($U = 8t$) correlated system, are considered. Results for the FLF-HF and FLF-DMFT calculations are compared to their parental approximations and to the reference lattice quantum Monte Carlo (QMC) data. At $h = 0$ the susceptibility tensor $\partial_{\mathbf{h}} \mathbf{m}$ is isotropic. Its diagonal component is equal to $\frac{1}{3} \partial_{h^l h^l} \ln \mathcal{Z}$, where the factor 1/3 compensates for the summation over the index l . The explicit relation for the FLF-HF theory can be found using the corresponding partition function \mathcal{Z}_{FLF} (13). The second derivative of the partition function then reads

$$\frac{\partial^2 \mathcal{Z}_{\text{FLF}}}{\partial h^l \partial h^l} = \int \left(\left[\frac{\partial \mathcal{S}_{\text{FLF}}[V]}{\partial h^l} \right]^2 - \frac{\partial^2 \mathcal{S}_{\text{FLF}}[V]}{\partial h^l \partial h^l} \right) e^{-\mathcal{S}_{\text{FLF}}[V]} \mathbf{V}^2 dV. \quad (25)$$

Derivatives at the right-hand side of this equation are obtained numerically. Note that in the absence of the external field h , the problem becomes isotropic, and the integral over the vector field V reduces to a single-variable integral over the absolute value of V . FLF-DMFT calculations start with obtaining self-energies for a polarized and nonpolarized DMFT solution. For this aim we use the exact diagonalization solver and apply $h = 0.005t$ as a small polarizing field. This allows us to obtain J_Q and L_Q quantities according to the above described procedure. Further calculations are performed in the same way as for the FLF-HF theory.

Let us turn to a comparison of obtained numerical results for all mentioned theories against a benchmark QMC result. Figure 3 shows an effective AFM Curie constant C as a function of an inverse temperature β for a 4×4 plaquette for $U = 2t$ (top panels) and $U = 8t$ (bottom panels). The left column corresponds to the HF case, and the right column shows the result obtained within DMFT scheme. The QMC data demonstrate that when lowering the temperature the Curie

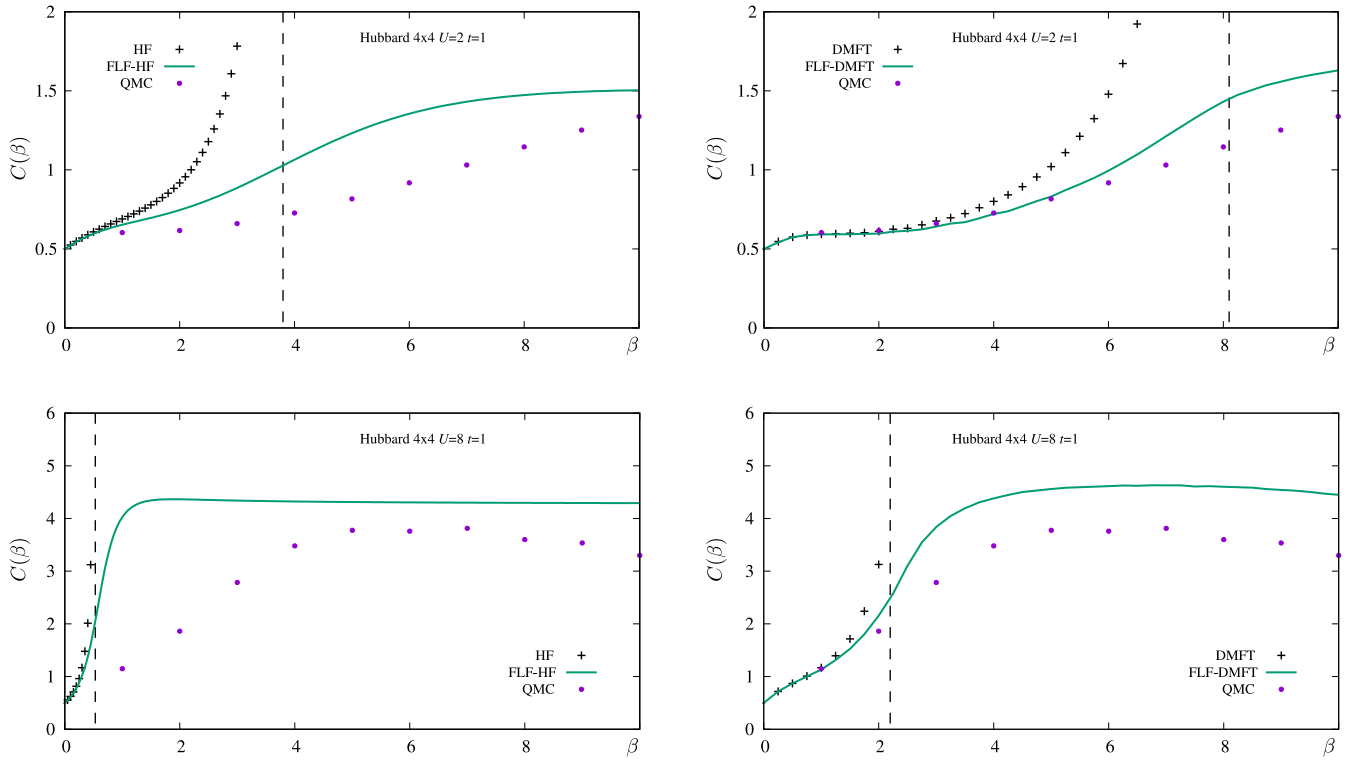


FIG. 3. Curie constant $C(\beta)$ as a function of the inverse temperature β calculated for 4×4 Hubbard plaquettes with periodic boundary conditions for $U = 2t$ (top panels) and $U = 8t$ (bottom panels). Results are obtained within HF (left column) and DMFT (right column) schemes. QMC reference data are depicted by purple dots, mean-field (HF and DMFT) results are shown by black pluses, and the FLF approach corresponds to the solid green line. The vertical dashed line indicates the mean-field Néel transition.

constant first increases. This corresponds to the formation and softening of a collective AFM mode. At a certain point $C(\beta)$ saturates, which is clearly visible in a strongly interacting regime. For very low temperatures that are not shown in the figure, $C(\beta)$ is expected to decay as $\beta^{-1}\chi_{gs}$ with χ_{gs} being the ground state susceptibility of the system.

We observe that the HF result agrees with the reference data only for a very high temperature. Lowering the temperature, the HF drastically overestimates the Curie constant and shows an unphysical (artificial) phase transition. The HF Néel point is indicated in Fig. 3 by a vertical dashed line. We note that a significant overestimation is seen already for temperatures far above the Néel point. Thus, we find that the applicability of the HF approximation is very limited even for a moderately correlated case, $U = 2t$. Compared to the HF method, DMFT leads to a quantitatively much better result for the Curie constant. In particular, the Néel temperature predicted by DMFT in a strongly correlated regime, $U = 8t$, is several times lower than the one of the HF. However the qualitative behavior of $C(\beta)$ at low temperatures remains the same.

The FLF extension dramatically improves the result of both mean-field approaches. For instance, a precise account for AFM fluctuations allows to prevent a spontaneous symmetry breaking associated with the AFM ordering. It is important to point out that, although the FLF calculations use the mean-field data as a starting point, resulting FLF curves for $C(\beta)$ remain smooth at Néel temperatures predicted by bare

mean-field theories. We find that FLF theories are in a good agreement with benchmark QMC data, especially for the FLF-DMFT calculations. Thus, the high-temperature region, where the FLF-DMFT approximation reproduces QMC points, is remarkably larger compared to the bare DMFT case. At lower temperatures, we observe a uniform discrepancy of about 20% between the FLF-DMFT and QMC results.

As a next step, let us demonstrate how the FLF-DMFT theory performs for larger plaquettes containing 6×6 and 8×8 lattice sites, and for a wider range of temperatures including the region way below the DMFT Néel point. Corresponding results are shown in Fig. 4. Here, we limit ourselves to a moderately interacting case of $U = 2t$, mostly because in this regime the reference QMC data can be obtained without heavy numerical efforts. At the same time, we stress that correlation effects at $U = 2t$ are by no means weak. This can be concluded from the fact that the Néel temperature predicted by DMFT is more than two times lower than the one of the HF theory (see Fig. 3). More elaborate studies also confirm that electron correlations become important at $U = 2t$ [61,73]. Indeed, although in this case the on-site Coulomb potential U is much smaller than the bandwidth $W = 8t$, the value of U should rather be compared to the width of a much narrower peak formed at the Fermi level in the electronic density of states.

As can be seen from the reference QMC data presented in Fig. 4, the change in the plaquette size results in two effects. First, the initial increase of the Curie constant upon

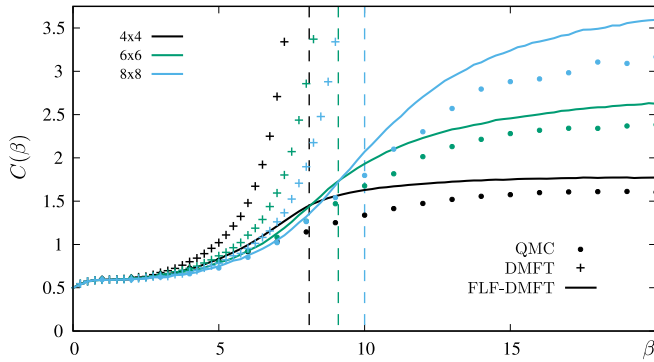


FIG. 4. Curie constant $C(\beta)$ obtained for $U = 2t$ for 4×4 (black), 6×6 (green), and 8×8 (blue) plaquettes as a function of the inverse temperature β . The results are compared for different QMC (dots), FLF-DMFT (solid line), and DMFT (crosses) approaches. The vertical dashed lines depict the DMFT Néel point, which depends on the size of plaquettes.

decreasing the temperature is slower for larger lattices. This trend is especially visible for a temperature range $4 \lesssim \beta \lesssim 8$ and is related to the local density of electronic states. Bare DMFT calculations qualitatively capture this effect. The same mechanism is responsible for a decrease of the DMFT Néel temperature upon increasing the plaquette size. The second effect is a significant increase of the Curie constant with the plaquette size below the DMFT Néel temperatures. However, this temperature range lies beyond the limit of applicability of DMFT. We emphasise that the DMFT Néel point or a slightly lower temperature is also a practical limitation for diagrammatic schemes constructed around DMFT [61].

Before switching to FLF-DMFT results, let us discuss what kind of change in the FLF data can be expected upon increasing the plaquette size. First, for larger plaquettes the AFM mode, which is associated with the wave vector $Q = (\pi, \pi)$, affects more lattice sites and thus becomes “more classical.” The fact that the FLF considers only classical fluctuations of the order parameter makes this method more appropriate for plaquettes that are not too small. However, for very large plaquettes other spatial fluctuations of the order parameter associated with $\mathbf{q} \neq Q$ become important. This argument is confirmed by the QMC result for the imaginary time dependence of the magnetic susceptibility $\chi_{\mathbf{q}}(\tau)$. In Fig. 5 the AFM component of the susceptibility obtained for $\mathbf{q} = Q$ (solid line) is compared to the local susceptibility summed over all wave vectors $N\chi_{loc}(\tau) = \sum_{\mathbf{q}} \chi_{\mathbf{q}}(\tau)$ (dotted line). The result is presented for $\beta = 20$, which is well below the DMFT Néel point. The FLF-DMFT predictions are indicated by dashed horizontal lines. First of all we observe that, except for a high-energy tails seen near $\tau = 0$ and $\tau = \beta$, the AFM susceptibility indeed shows a weak τ dependence for all considered lattices. Also, we find that at $\tau = \beta/2$ the value of $N\chi_{loc}$ is very close to χ_Q . This proves that the low-energy collective fluctuations are dominated by a single AMF mode associated with the $Q = (\pi, \pi)$ and $\Omega = 0$ channel, which justifies the main idea of the FLF approach. It can be seen that deviation of $N\chi_{loc}(\tau)$ from $\chi_Q(\tau)$ grows with the lattice size, indicating that contributions of other $\mathbf{q} \neq Q$ fluctuations be-

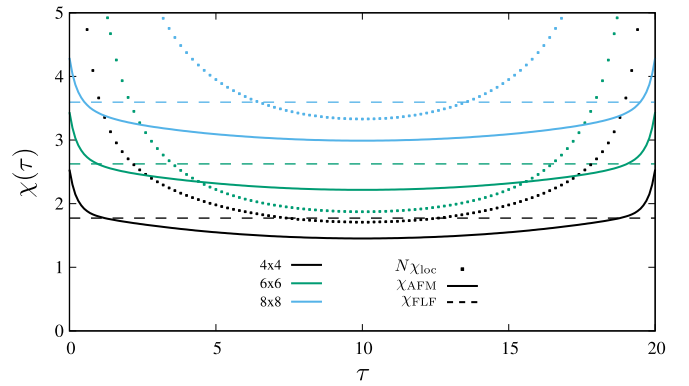


FIG. 5. Magnetic susceptibility $\chi(\tau)$ calculated for 4×4 (black), 6×6 (green), and 8×8 (blue) plaquettes as a function of the imaginary time τ . Local (dots) and AFM (solid lines) susceptibilities are exact QMC results. Horizontal dashed lines correspond to the FLF-DMFT approximation.

come more important. This analysis suggests that FLF-DMFT approach is best suited for medium plaquettes.

Figure 4 confirms the above reasoning. Indeed, among all plaquettes the best numerical accuracy of the FLF-DMFT is observed for the 6×6 system. For the 4×4 plaquette, the biggest deviation from the benchmark result is observed near the DMFT Néel point, where a Mexican hat potential starts to form. It can be concluded that quantum fluctuations of the order parameter are particularly important in this regime. On the other hand, the biggest overestimation of the Curie constant for the 8×8 plaquette is observed at low temperatures. As we have discussed above, such an overestimation is associated with neglecting uncorrelated spatial fluctuations of the order parameter. It can be seen that the FLF-DMFT method in its present form reduces to bare DMFT in the limit of an infinite lattice, because the saddle-point estimation of the integral over the FLF becomes exact. Since the DMFT predicts a divergence in the Curie constant, the FLF-DMFT is expected to show a larger overestimation of C for bigger plaquettes.

Nevertheless, the overall performance of the FLF-DMFT approach and its agreement with the reference data are found to be quite satisfactory. In fact, below the DMFT Néel point T_N^{DMFT} the discrepancy between the FLF-DMFT and reference QMC data does not exceed 20% for all considered plaquettes. Moreover, this difference remains almost unchanged even for very low temperatures $T \simeq 0.5 T_N^{\text{DMFT}}$. Note that this regime of temperatures is known to be extremely difficult for numerical calculations, because even the most advanced theoretical approaches are not able to provide reasonable results below $T \simeq 0.75 T_N^{\text{DMFT}}$ [61]. In this regard, we can qualitatively compare the result of the FLF-DMFT theory for the 8×8 plaquette with the results of existing theories obtained for the infinite lattice. One finds that, enlarging the lattice size from 8×8 to infinity, the DMFT Néel temperature decreases from $T = 0.10t$ to $T = 0.08t$. Then, for the same value of the on-site Coulomb potential $U = 2t$ considered in our work, we observe that the exact diagrammatic Monte Carlo (DiagMC) methods [55,74] do not converge below $T = 0.83 T_N^{\text{DMFT}}$. The dual fermion [38,75–77] and

the dual boson [41–45] approaches quantitatively agree with the DiagMC result for magnetic susceptibility, but are limited to the temperature range $T \gtrsim 0.78 T_N^{\text{DMFT}}$ (see Fig. 13 of Ref. [61]). Diagrammatic extensions of DMFT such as the dynamical vertex approximation (D Γ A) [39,40] and the TRILEX theory [34–36] can perform calculations for lower temperatures $T \simeq 0.75 T_N^{\text{DMFT}}$ and $T \simeq 0.63 T_N^{\text{DMFT}}$, respectively. However, at the DMFT Néel point both theories deviate from the exact result already by 10–15%, and this accuracy rapidly decays to 30–50% when lowering the temperature. In contrast, the FLF-DMFT result for the 8×8 plaquette presented in Fig. 4 shows a uniform discrepancy of about 10–15% down to the lowest considered temperature, that is $T = 0.5 T_N^{\text{DMFT}}$. This illustrates a conceptual advantage of the FLF method that exactly accounts for strong AFM fluctuations, which cause problems for all existing diagrammatic extensions of DMFT.

IV. CONCLUSIONS AND OUTLOOK

We have demonstrated that an accurate account for fluctuations of soft collective modes is crucially important for a correct description of a low-temperature behavior of correlated electronic systems. For this reason we have introduced and tested a fluctuating local field technique, which is capable of handling these collective modes in a wide temperature range, including a strongly nonlinear regime of fluctuations. Compared to an exact QMC solution for half-filled Hubbard plaquettes, the FLF-DMFT scheme shows a quantitatively good result for the Curie constant. The reason is that FLF-DMFT explicitly considers collective AFM fluctuations in addition to local correlations accounted for by a bare DMFT approach.

In the present paper we have benchmarked the FLF theory for a half-filled Hubbard plaquettes with emerging classical fluctuations of a single collective AFM mode. This system has been chosen because of its conceptual simplicity, availability of the numerically exact reference data, and, simultaneously, a clear lack of existing approximations that can provide a satisfactory solution at low temperature. The FLF-DMFT approach shows an accuracy of about 20% or better for all considered regimes including the temperature twice lower than the DMFT Néel point. We consider these results rather promising, bearing in mind that the introduced computational scheme does not require significant numerical efforts beyond DMFT calculations.

In its present form the FLF method can be straightforwardly applied to a wide range of finite correlated systems that exhibit strong collective (charge, spin, etc.) fluctuations with dominant single or few collective modes. In particular, molecular magnets can be seen as attractive candidates for the first realistic application of the FLF theory. Technically, leading collective modes can be determined from the instabilities and/or multiple solutions that arise from the mean-field consideration. For example, one can propose a single-stripe solution for the $L_x \times L_y$ Hubbard plaquette away from the half-filling by imposing fluctuations in the $(\pi - 2\pi/L_x, \pi)$ channel. Of course, a quantitative accuracy of this scheme requires an additional consideration. On the other hand, modeling of large 2D lattices would require an extension of the theory towards an inclusion of other than AFM spatial

fluctuating modes. This problem can be addressed, for example, by modeling the infinite lattice within a cluster scheme, and using the FLF method as a cluster solver. However, this would require an additional study of whether the FLF can produce sufficiently accurate data for the Green’s function. A possible improvement of the numerical accuracy of the FLF-DMFT method can be achieved by using a better reference system. Here, we can benefit from the fact that the introduced scheme is based on the dual fermion ideology and thus is not restricted only to the single-site impurity problem of DMFT [77]. Then, the use of a small, e.g., 2×2 cluster as the reference system will allow to us consider short-range correlations exactly, whereas the collective AFM fluctuations can be accounted for by the fluctuating field. Importantly, the FLF method can be formulated for all possible cluster schemes, such as a free-standing cluster or a cluster with periodic boundary conditions [72,78]. For this purpose, the impurity Green’s function and hybridization in the FLF-DMFT equations should be simply replaced by corresponding quantities of the cluster scheme.

In a broader context, it is worthwhile to relate our method to other known approaches that handle strong fluctuations in quantum systems. Whenever leading fluctuating degrees of freedom can be clearly isolated, constrained calculations are widely used. For example, the analysis of molecular conformations in quantum chemistry is essentially based on the estimation of the electronic energy for a constrained atomic configuration [79]. However, there is no good way to introduce a constraint for collective degrees of freedom, for instance, to keep the total magnetization fixed while allowing for single-electron excitations. Instead, in our work we have introduced an additional variable, namely the fluctuating field V , that affects the *average* value of the order parameter. It resembles a seminal approach by Wheeler *et al.* known as the generator coordinate method [80,81]. It is widely used in the field of nuclear physics, and also has proved its efficiency in a number of developments including quantum chemistry [82]. This variational approach works with a set of configurations that differ by the value of the field acting on the system. In practice, only a few configurations are considered, otherwise the method becomes computationally expensive. This is the most obvious difference from the FLF theory, where the integral is taken over a continuously varied fluctuating field, which in particular allows us to respect the spin-rotation symmetry. Another prominent link can be established to the contemporary field theories based on the functional renormalization group (fRG) [83]. This method relies on the generating functional $W(V) = \ln \int D[\phi] \exp\{-S[\phi] + V\phi\}$, where the action $S[\phi]$ describes the nonlinear bosonic field theory. Thus, the FLF-HF can be seen as a generalization of the previously known methods [80–83]. On the other hand, the unique advantage of the FLF-DMFT scheme over other known approaches is that it allows for a simultaneous unperturbative treatment of the on-site correlations together with spatial fluctuations of the “global” order parameter.

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- [1] A. Kamal, *Nuclear Physics* (Springer, Berlin, 2014).
- [2] J. W. Abraham and M. Bonitz, Quantum breathing mode of trapped particles: From nanoplasmas to ultracold gases, *Contrib. Plasma Phys.* **54**, 27 (2014).
- [3] D. Greif, T. Uehlinger, G. Jotzu, L. Tarruell, and T. Esslinger, Short-range quantum magnetism of ultracold fermions in an optical lattice, *Science* **340**, 1307 (2013).
- [4] R. A. Hart, P. M. Duarte, T.-Lin Yang, X. Liu, T. Paiva, E. Khatami, R. T. Scalettar, N. Trivedi, D. A. Huse, and R. G. Hulet, Observation of antiferromagnetic correlations in the Hubbard model with ultracold atoms, *Nature (London)* **519**, 211 (2015).
- [5] D. Greif, G. Jotzu, M. Messer, R. Desbuquois, and T. Esslinger, Formation and Dynamics of Antiferromagnetic Correlations in Tunable Optical Lattices, *Phys. Rev. Lett.* **115**, 260401 (2015).
- [6] L. W. Cheuk, M. A. Nichols, K. R. Lawrence, M. Okan, H. Zhang, E. Khatami, N. Trivedi, T. Paiva, M. Rigol, and M. W. Zwierlein, Observation of spatial charge and spin correlations in the 2D Fermi-Hubbard model, *Science* **353**, 1260 (2016).
- [7] N. Blanc, J. Trinh, L. Dong, X. Bai, A. A. Aczel, M. Mourigal, L. Balents, T. Siegrist, and A. P. Ramirez, Quantum criticality among entangled spin chains, *Nat. Phys.* **14**, 273 (2018).
- [8] E. Coronado, Molecular magnetism: from chemical design to spin control in molecules, materials and devices, *Nat. Rev. Mater.* **5**, 87 (2019).
- [9] M. Holynska, *Single-Molecule Magnets: Molecular Architectures and Building Blocks for Spintronics* (John Wiley & Sons, New York, 2019).
- [10] E. Fradkin, *Field Theories of Condensed Matter Systems* (Westview, Oxford, 1997).
- [11] D. Sénéchal, A. M. Tremblay, and C. Bourbonnais, *Theoretical Methods for Strongly Correlated Electrons* (Springer, Berlin, 2006).
- [12] M. V. You and V. Heine, Magnetism in transition metals at finite temperatures. I. Computational model, *J. Phys. F* **12**, 177 (1982).
- [13] A. J. Holden and M. V. You, Magnetism in transition metals at finite temperatures. II. Application to the thermodynamic excitations in iron: spin waves and TC, *J. Phys. F* **12**, 195 (1982).
- [14] J. Hubbard, The magnetism of iron, *Phys. Rev. B* **19**, 2626 (1979).
- [15] J. Hubbard, Magnetism of iron. II, *Phys. Rev. B* **20**, 4584 (1979).
- [16] B. I. Shraiman and E. D. Siggia, Mobile Vacancies in a Quantum Heisenberg Antiferromagnet, *Phys. Rev. Lett.* **61**, 467 (1988).
- [17] H. J. Schulz, Effective Action for Strongly Correlated Fermions from Functional Integrals, *Phys. Rev. Lett.* **65**, 2462 (1990).
- [18] Z. Y. Weng, C. S. Ting, and T. K. Lee, Path-integral approach to the Hubbard model, *Phys. Rev. B* **43**, 3790 (1991).
- [19] M. S. Scheurer, S. Chatterjee, W. Wu, M. Ferrero, A. Georges, and S. Sachdev, Topological order in the pseudogap metal, *Proc. Natl. Acad. Sci. USA* **115**, E3665 (2018).
- [20] C. Zhou and H. J. Schulz, Quantum fluctuations in the spiral phase of the Hubbard model, *Phys. Rev. B* **52**, R11557 (1995).
- [21] H. J. Schulz, Functional integrals for correlated fermions, *J. Low Temp. Phys.* **99**, 615 (1995).
- [22] G. Rohringer, H. Hafermann, A. Toschi, A. A. Katanin, A. E. Antipov, M. I. Katsnelson, A. I. Lichtenstein, A. N. Rubtsov, and K. Held, Diagrammatic routes to nonlocal correlations beyond dynamical mean field theory, *Rev. Mod. Phys.* **90**, 025003 (2018).
- [23] J. C. Slater, Note on Hartree’s method, *Phys. Rev.* **35**, 210 (1930).
- [24] V. Fock, Näherungsmethode zur lösung des quantenmechanischen mehrkörperproblems, *Z. Phys.* **61**, 126 (1930).
- [25] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions, *Rev. Mod. Phys.* **68**, 13 (1996).
- [26] J. Gukelberger, L. Huang, and P. Werner, On the dangers of partial diagrammatic summations: Benchmarks for the two-dimensional Hubbard model in the weak-coupling regime, *Phys. Rev. B* **91**, 235114 (2015).
- [27] P. Sun and G. Kotliar, Extended dynamical mean-field theory and GW method, *Phys. Rev. B* **66**, 085120 (2002).
- [28] S. Biermann, F. Aryasetiawan, and A. Georges, First-Principles Approach to the Electronic Structure of Strongly Correlated Systems: Combining the GW Approximation and Dynamical Mean-Field Theory, *Phys. Rev. Lett.* **90**, 086402 (2003).
- [29] T. Ayrál, P. Werner, and S. Biermann, Spectral Properties of Correlated Materials: Local Vertex and Nonlocal Two-Particle Correlations from Combined GW and Dynamical Mean Field Theory, *Phys. Rev. Lett.* **109**, 226401 (2012).
- [30] T. Ayrál, S. Biermann, and P. Werner, Screening and non-local correlations in the extended Hubbard model from self-consistent combined GW and dynamical mean field theory, *Phys. Rev. B* **87**, 125149 (2013).
- [31] L. Huang, T. Ayrál, S. Biermann, and P. Werner, Extended dynamical mean-field study of the Hubbard model with long-range interactions, *Phys. Rev. B* **90**, 195114 (2014).
- [32] L. Boehnke, F. Nilsson, F. Aryasetiawan, and P. Werner, When strong correlations become weak: Consistent merging of GW and DMFT, *Phys. Rev. B* **94**, 201106(R) (2016).
- [33] T. Ayrál, S. Biermann, P. Werner, and L. Boehnke, Influence of Fock exchange in combined many-body perturbation and dynamical mean field theory, *Phys. Rev. B* **95**, 245130 (2017).
- [34] T. Ayrál and O. Parcollet, Mott physics and spin fluctuations: A unified framework, *Phys. Rev. B* **92**, 115109 (2015).
- [35] T. Ayrál and O. Parcollet, Mott physics and spin fluctuations: A functional viewpoint, *Phys. Rev. B* **93**, 235124 (2016).
- [36] T. Ayrál, J. Vučković, and O. Parcollet, Fierz Convergence Criterion: A Controlled Approach to Strongly Interacting Systems with Small Embedded Clusters, *Phys. Rev. Lett.* **119**, 166401 (2017).

- [37] E. A. Stepanov, V. Harkov, and A. I. Lichtenstein, Consistent partial bosonization of the extended Hubbard model, *Phys. Rev. B* **100**, 205115 (2019).
- [38] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Dual fermion approach to nonlocal correlations in the hubbard model, *Phys. Rev. B* **77**, 033101 (2008).
- [39] A. Toschi, A. A. Katanin, and K. Held, Dynamical vertex approximation: A step beyond dynamical mean-field theory, *Phys. Rev. B* **75**, 045118 (2007).
- [40] A. A. Katanin, A. Toschi, and K. Held, Comparing pertinent effects of antiferromagnetic fluctuations in the two- and three-dimensional Hubbard model, *Phys. Rev. B* **80**, 075104 (2009).
- [41] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Dual boson approach to collective excitations in correlated fermionic systems, *Ann. Phys. (NY)* **327**, 1320 (2012).
- [42] E. G. C. P. van Loon, A. I. Lichtenstein, M. I. Katsnelson, O. Parcollet, and H. Hafermann, Beyond extended dynamical mean-field theory: Dual boson approach to the two-dimensional extended Hubbard model, *Phys. Rev. B* **90**, 235135 (2014).
- [43] E. A. Stepanov, E. G. C. P. van Loon, A. A. Katanin, A. I. Lichtenstein, M. I. Katsnelson, and A. N. Rubtsov, Self-consistent dual boson approach to single-particle and collective excitations in correlated systems, *Phys. Rev. B* **93**, 045107 (2016).
- [44] E. A. Stepanov, A. Huber, E. G. C. P. van Loon, A. I. Lichtenstein, and M. I. Katsnelson, From local to nonlocal correlations: The dual boson perspective, *Phys. Rev. B* **94**, 205110 (2016).
- [45] L. Peters, E. G. C. P. van Loon, A. N. Rubtsov, A. I. Lichtenstein, M. I. Katsnelson, and E. A. Stepanov, Dual boson approach with instantaneous interaction, *Phys. Rev. B* **100**, 165128 (2019).
- [46] G. V. Astretsov, G. Rohringer, and A. N. Rubtsov, Dual parquet scheme for the two-dimensional Hubbard model: Modeling low-energy physics of high- T_c cuprates with high momentum resolution, *Phys. Rev. B* **101**, 075109 (2020).
- [47] S. Isakov, A. E. Antipov, and E. Gull, Diagrammatic Monte Carlo for dual fermions, *Phys. Rev. B* **94**, 035102 (2016).
- [48] J. Gukelberger, E. Kozik, and H. Hafermann, Diagrammatic monte carlo approach for diagrammatic extensions of dynamical mean-field theory: Convergence analysis of the dual fermion technique, *Phys. Rev. B* **96**, 035152 (2017).
- [49] M. Vandelli, V. Harkov, E. A. Stepanov, J. Gukelberger, E. Kozik, A. Rubio, and A. I. Lichtenstein, Dual boson diagrammatic Monte Carlo approach applied to the extended Hubbard model, *Phys. Rev. B* **102**, 195109 (2020).
- [50] E. G. C. P. van Loon, H. Hafermann, A. I. Lichtenstein, A. N. Rubtsov, and M. I. Katsnelson, Plasmons in Strongly Correlated Systems: Spectral Weight Transfer and Renormalized Dispersion, *Phys. Rev. Lett.* **113**, 246407 (2014).
- [51] H. Hafermann, E. G. C. P. van Loon, M. I. Katsnelson, A. I. Lichtenstein, and O. Parcollet, Collective charge excitations of strongly correlated electrons, vertex corrections, and gauge invariance, *Phys. Rev. B* **90**, 235105 (2014).
- [52] E. G. C. P. van Loon, M. Rösner, G. Schönhoff, M. I. Katsnelson, and T. O. Wehling, Competing Coulomb and electron-phonon interactions in NbS₂, *npj Quantum Mater.* **3**, 32 (2018).
- [53] E. A. Stepanov, L. Peters, I. S. Krivenko, A. I. Lichtenstein, M. I. Katsnelson, and A. N. Rubtsov, Quantum spin fluctuations and evolution of electronic structure in cuprates, *npj Quantum Mater.* **3**, 54 (2018).
- [54] N. D. Mermin and H. Wagner, Absence of Ferromagnetism or Antiferromagnetism in One- or Two-Dimensional Isotropic Heisenberg Models, *Phys. Rev. Lett.* **17**, 1133 (1966).
- [55] N. V. Prokof'ev and B. V. Svistunov, Polaron Problem by Diagrammatic Quantum Monte Carlo, *Phys. Rev. Lett.* **81**, 2514 (1998).
- [56] E. Kozik, K. V. Houcke, E. Gull, L. Pollet, N. Prokof'ev, B. Svistunov, and M. Troyer, Diagrammatic Monte Carlo for correlated fermions, *Europhys. Lett.* **90**, 10004 (2010).
- [57] R. Rossi, Determinant Diagrammatic Monte Carlo Algorithm in the Thermodynamic Limit, *Phys. Rev. Lett.* **119**, 045701 (2017).
- [58] R. Rossi, F. Werner, N. Prokof'ev, and B. Svistunov, Shifted-action expansion and applicability of dressed diagrammatic schemes, *Phys. Rev. B* **93**, 161102(R) (2016).
- [59] F. Šimkovic and E. Kozik, Determinant Monte Carlo for irreducible Feynman diagrams in the strongly correlated regime, *Phys. Rev. B* **100**, 121102(R) (2019).
- [60] R. Rossi, Direct sampling of the self-energy with connected determinant Monte Carlo, [arXiv:1802.04743](https://arxiv.org/abs/1802.04743).
- [61] T. Schäfer, N. Wentzell, I. Šimkovic, Fedor, Y.-Y. He, C. Hille, M. Klett, C. J. Eckhardt, B. Arzhang, V. Harkov, F.-M. Le Régent, A. Kirsch, Y. Wang, A. J. Kim, E. Kozik, E. A. Stepanov, A. Kauch, S. Andergassen, P. Hansmann, D. Rohe, Y. M. Vilk, J. P. F. LeBlanc, S. Zhang, A. M. S. Tremblay, M. Ferrero, O. Parcollet, and A. Georges, Tracking the footprints of spin fluctuations: A multi-method, multi-messenger study of the two-dimensional Hubbard model, [arXiv:2006.10769](https://arxiv.org/abs/2006.10769).
- [62] E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, Sign problem in the numerical simulation of many-electron systems, *Phys. Rev. B* **41**, 9301 (1990).
- [63] W. Wu, M. Ferrero, A. Georges, and E. Kozik, Controlling Feynman diagrammatic expansions: Physical nature of the pseudogap in the two-dimensional Hubbard model, *Phys. Rev. B* **96**, 041105(R) (2017).
- [64] A. N. Rubtsov, Fluctuating local field method probed for a description of small classical correlated lattices, *Phys. Rev. E* **97**, 052120 (2018).
- [65] J. Jaeckel and C. Wetterich, Flow equations without mean field ambiguity, *Phys. Rev. D* **68**, 025020 (2003).
- [66] T. Baier, E. Bick, and C. Wetterich, Temperature dependence of antiferromagnetic order in the Hubbard model, *Phys. Rev. B* **70**, 125111 (2004).
- [67] J. Jaeckel, Understanding the Fierz ambiguity of partially bosonized theories, [arXiv:hep-ph.0205154](https://arxiv.org/abs/hep-ph.0205154).
- [68] R. Peierls, On a minimum property of the free energy, *Phys. Rev.* **54**, 918 (1938).
- [69] N. N. Bogolyubov, A variation principle in the problem of many bodies, *Dokl. Akad. Nauk SSSR* **119**, 244 (1958).
- [70] R. P. Feynman, *Statistical Mechanics* (Benjamin, Reading, MA, 1972).
- [71] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevB.102.224423> for the variational derivation of the FLF-HF method and for the path-integral derivation of the FLF-DMFT theory.
- [72] G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Electronic structure calculations

- with dynamical mean-field theory, *Rev. Mod. Phys.* **78**, 865 (2006).
- [73] A. J. Kim, F. Simkovic, and E. Kozik, Spin and Charge Correlations across the Metal-to-Insulator Crossover in the Half-Filled 2D Hubbard Model, *Phys. Rev. Lett.* **124**, 117602 (2020).
- [74] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Monte Carlo calculations of coupled boson-fermion systems. I, *Phys. Rev. D* **24**, 2278 (1981).
- [75] A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and A. Georges, Dual fermion approach to the two-dimensional Hubbard model: Antiferromagnetic fluctuations and Fermi arcs, *Phys. Rev. B* **79**, 045133 (2009).
- [76] H. Hafermann, G. Li, A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and H. Monien, Efficient Perturbation Theory for Quantum Lattice Models, *Phys. Rev. Lett.* **102**, 206401 (2009).
- [77] S. Brener, E. A. Stepanov, A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Dual fermion method as a prototype of generic reference-system approach for correlated fermions, *Ann. Phys. (NY)* **422**, 168310 (2020).
- [78] T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Quantum cluster theories, *Rev. Mod. Phys.* **77**, 1027 (2005).
- [79] P. G. Szalay, T. Müller, G. Gidofalvi, H. Lischka, and R. Shepard, Multiconfiguration self-consistent field and multireference configuration interaction methods and applications, *Chem. Rev.* **112**, 108 (2012).
- [80] D. L. Hill and J. A. Wheeler, Nuclear constitution and the interpretation of fission phenomena, *Phys. Rev.* **89**, 1102 (1953).
- [81] J. J. Griffin and J. A. Wheeler, Collective motions in nuclei by the method of generator coordinates, *Phys. Rev.* **108**, 311 (1957).
- [82] K. Capelle, Variational calculation of many-body wave functions and energies from density functional theory, *J. Chem. Phys.* **119**, 1285 (2003).
- [83] J. Polonyi, Lectures on the functional renormalization group method, *Central Eur. J. Phys.* **1**, 1 (2003).