

Magnetic instabilities in three- and higher-dimensional Hubbard models with different lattice geometries: Impact of nonlocal spatial correlations

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We analyze the impact of the lattice geometry on the thermodynamic transition to magnetically ordered phases in strongly interacting electron systems for various Bravais lattices in three, four, and five dimensions, including both local and nonlocal correlation effects. In a first step we use the dynamical mean-field theory (DMFT), which takes into account purely local correlations, to calculate the magnetic susceptibilities of the Hubbard model on three- (3d-sc), four- (4d-sc), and five- dimensional (5d-sc) simple cubic/hypercubic, as well as on three- dimensional body- (bcc) and face-centered (fcc) cubic lattices, and determine the transition temperature to the corresponding magnetically ordered state. In a second step, we exploit the dynamical vertex approximation (DΓA), a diagrammatic extension of DMFT, to include the effect of nonlocal correlations which are particularly important in the vicinity of the corresponding phase transition. For the bipartite 3d-sc, 4d-sc, 5d-sc, and bcc lattices nonlocal fluctuations lead to a substantial reduction of the DMFT transition temperature consistent to the overall tendency of mean-field approaches to overestimate the stability of ordered phases. As expected, the magnitude of the difference between the DMFT, being exact in the limit of large connectivity/dimensions, and DΓA transition temperatures decreases with increasing coordination number. On a more practical perspective, these results also provide a reasonable guidance to evaluate the expected overestimation of the DMFT ordering temperature for different material geometries. For the fcc lattice, on the other hand, the ordered phase observed in DMFT vanishes completely within DΓA which is consistent with the existence of strong geometric frustration in this lattice.

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I. INTRODUCTION

The properties of crystalline materials are determined by two main ingredients, namely the type of periodic lattice, which is formed by the atomic ions and the interaction between the electrons which move in this positively charged background. Even if we consider a static lattice within the well-known Born-Oppenheimer approximation [1], which acts as a stage for the dynamics of the electrons, the resulting many-body problem is still very hard to tackle theoretically. In this situation it is of uttermost importance to select the appropriate numerical (or analytical) tools for the theoretical analysis. The actual choice is dictated by the relative importance of the two main above-mentioned ingredients for the given system, i.e., the structure of the lattice and the interaction between the electrons. In the case of sufficiently weak

interactions the physics is dominated by the structure of the underlying lattice and can be captured by low-order perturbation theory such as GW [2,3] or by an effective single-particle description as provided by density functional theory [4,5]. The electronic state is typically well described by Bloch wave functions and the electrons are completely delocalized over the entire lattice. In the opposite limit, where the interaction between two electrons at one lattice site is much larger than the corresponding tunneling probability between the lattice sites, the electronic charge becomes localized in real space forming, for instance, a correlation-driven (Mott) insulating state. Strong-coupling perturbation theory [6,7] is one of the methods which can treat this situation quite well, being obviously not adequate for the metallic side of the system. The intermediate case, where both the lattice structure as well as the interactions between the electrons are equally relevant, is the most challenging situation for the theoretical treatment of a many-body problem.

In this respect, the dynamical mean-field theory [8–11] (DMFT) has represented a huge step forward as it is able to capture all purely local correlations of interacting lattice electrons, allowing for a unified description of the entire

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coupling regime. Among the biggest successes of DMFT are the accurate quantitative description of the correlation-driven Mott metal-to-insulator transition in model systems such as the single-band Hubbard model [12–15] and real materials [16] such as transition metal oxides [17,18], the uncovering of orbital selective Mott transitions [19], the identification of peculiar correlation-driven features in the spectral function [20] and in the specific heat [21] or topological transitions without gap closing [22], the recently discovered orbital-magnetic-field-driven insulator-to-metal transition in the Hubbard-Hofstadter model [23]. Of particular interest are also the investigation of magnetic quantum phase transitions [24] and DMFT studies of magnetically ordered phases and the associated phase transitions which are difficult to tackle theoretically even at weak to intermediate coupling [25]. In fact, DMFT has advanced our understanding of the magnetism in iron and nickel [26,27] or the ferro-orbital order in LaTiO_3 [28]. On the model level, DMFT correctly captures the crossover from a weakly coupled Slater to a strongly coupled Heisenberg antiferromagnet in the single-band Hubbard model on a three-dimensional bipartite cubic lattice [29–31].

In spite of its achievements, DMFT has serious limitations where the most notable one is arguably its intrinsic inability to capture nonlocal correlation effects. This leads, for instance, to an overestimation of the transition temperature to magnetically ordered phases in three spatial dimensions [32] or the prediction of a spurious phase transition in two dimensions [33], which is forbidden by the Mermin-Wagner theorem [34]. To this end, diagrammatic extensions of DMFT [35] have been developed where a Feynman diagrammatic expansion around a correlated DMFT starting point is performed by constructing Feynman diagrams from the local vertex and nonlocal Green's functions of DMFT. In the last decade this idea has been used in various ways which led to the development of the dynamical vertex approximation (D Γ A) [36] in its parquet [37,38] and ladder [39–41] implementation, the dual fermion [42–45] and dual boson [46] methods, the one-particle irreducible approach [47] as well as the TRILEX [48,49] and QUADRILEX [50] methods. Within the ladder D Γ A nonlocal correlations sizably reduce the DMFT transition temperature to an antiferromagnetically ordered state in the three-dimensional bipartite Hubbard model [29,32] and lead to a suppression of the magnetically ordered state at any finite temperature on the two-dimensional square lattice in accordance with the Mermin-Wagner theorem [33].

In this paper, we extend these ladder D Γ A studies of the three-dimensional Hubbard model on a simple cubic lattice to various three-, four- and five-dimensional lattices to gain insights in the specific role played by lattice coordination and dimension on the magnetic transition. More specifically, we consider the body- and face-centered-cubic lattices in three dimensions as well as the simple (hyper)cubic lattices in three, four (tesseract), and five dimensions and compare their magnetic DMFT phase diagram for selected fillings to corresponding ladder D Γ A results. We find that, in general, the difference between DMFT and ladder D Γ A decreases with increasing coordination number and/or dimension which is indeed the expected behavior, as DMFT is known to perform better in higher dimensions (or, more generally, for systems with higher coordination number) and eventually becomes

exact in the limit of infinite coordination number [51]. Moreover, in four and five dimensions we simultaneously obtain, as expected, both a sizable reduction of T_N in ID Γ A with respect to DMFT as well as critical exponents compatible with the mean-field (MF) universality class (except for logarithmic corrections in four dimensions) which supports the overall reliability of the approach to study magnetic transitions of correlated electrons beyond MF/DMFT.

Apart from describing these general trends, we provide accurate values for the transition temperatures in the strong coupling Heisenberg regime, and compare them with the corresponding DMFT values. This can serve as an insightful guidance for a quick estimate (or prediction) of experimentally observed critical temperatures for different material geometries, based on purely DMFT results (e.g., in the situations where realistic calculations beyond DMFT are not feasible), as well as a reliable benchmark for future studies of the magnetically ordered phases of strongly correlated electrons.

Finally, we quantify the importance of nonlocal correlations by calculating the magnitude of the violation of specific sum rules within DMFT which originate from its inability to capture spatial fluctuations with the necessary accuracy.

The paper is organized as follows: In Sec. II we introduce the Hubbard model on the different lattices mentioned above and give a short overview about the ladder D Γ A approximation. In Sec. III, we present our results for the spin susceptibilities of both DMFT and ladder D Γ A, the critical exponent as well as the magnetic phase diagram for DMFT and D Γ A. We also discuss the phase transition at weak coupling and analyze how the violation of a specific sum rule within DMFT depends on the geometric structure of the lattice. Finally, in Sec. IV we summarize our results and discuss future research perspectives. In Appendix we present random phase approximation (RPA) results for the fcc lattice.

II. MODEL AND METHOD

For this study we consider the single-band Hubbard model

$$H = -t \sum_{\sigma(ij)} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}^\dagger$ annihilates (creates) an electron with spin σ at lattice site $\mathbf{R}_i$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the particle number, t denotes the hopping amplitude between nearest neighbors and U is the on-site Hubbard interaction. We will study this model on the following three-, four-, and five-dimensional lattices which are shown in Fig. 1 with increasing coordination number from left to right and increasing dimension from bottom to top: the simple-cubic lattice in three dimensions (lower row, left), the body-centered-cubic lattice (lower row, middle), the face-centered-cubic lattice (lower row, right) and the simple hypercubic lattice (upper row, middle) in four dimensions (tesseract), while the five-dimensional hypercubic lattice is only indicated by its coordination number. Let us note that for the representation of the $4d$ hypercubic lattice we have selected a projection to three dimensions where the coordination number of the lattice can be seen in the most transparent way [52,53]. We choose the hopping parameter t to fix the second

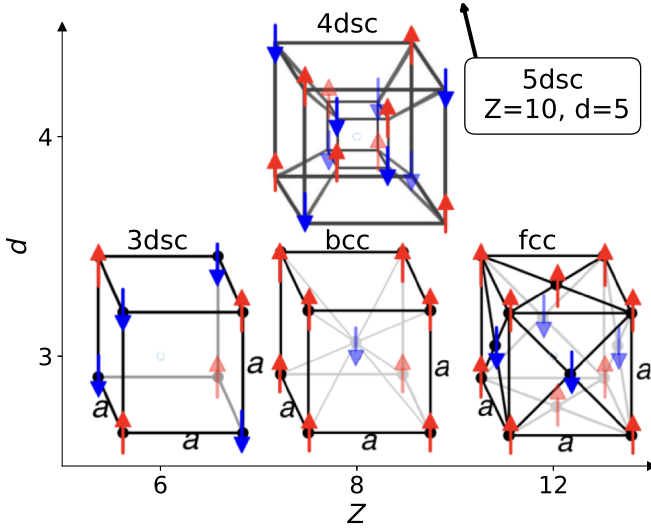


FIG. 1. Three-dimensional simple cubic (3d-sc), body-centered-cubic (bcc), face-centered-cubic (fcc) and four-dimensional simple cubic (4d-sc, tesseract) lattices considered in this study ordered by increasing coordination number Z (from left to right) and increasing spatial dimension d (from bottom to top). Since projections of the five-dimensional cubic lattice are barely recognizable on paper, it is only signified by its coordination number and dimension. Arrows display the spin arrangement for the predominant magnetic order.

moment of the noninteracting density of states to 0.5 which allows for a direct comparison between the different lattices in DMFT [54]. This implies that $t = 1/(2\sqrt{Z})$ where Z is the coordination number of the lattice (i.e., $Z_{\text{bcc}} = Z_{\text{4d-sc}} = 8$, $Z_{\text{5d-sc}} = 10$, $Z_{\text{fcc}} = 12$ to be compared with $Z_{\text{3d-sc}} = 6$). The tight-binding dispersion relations for each lattice are given by

$$\epsilon_{\text{3d-sc}} = -2t(\cos ak_x + \cos ak_y + \cos ak_z), \quad (2a)$$

$$\epsilon_{\text{bcc}} = -8t \cos \frac{ak_x}{2} \cos \frac{ak_y}{2} \cos \frac{ak_z}{2}, \quad (2b)$$

$$\epsilon_{\text{fcc}} = -4t \left(\cos \frac{ak_x}{2} \cos \frac{ak_y}{2} + \cos \frac{ak_x}{2} \cos \frac{ak_z}{2} + \cos \frac{ak_y}{2} \cos \frac{ak_z}{2} \right). \quad (2c)$$

$$\epsilon_{\text{4d-sc}} = -2t(\cos ak_1 + \cos ak_2 \quad (2d)$$

$$+ \cos ak_3 + \cos ak_4), \quad (2e)$$

$$\epsilon_{\text{5d-sc}} = -2t(\cos ak_1 + \cos ak_2 + \cos ak_3 + \cos ak_4 + \cos ak_5), \quad (2f)$$

where we set $a = 1$. In the following, we denote fermionic Matsubara frequencies with $\nu_n = (2n + 1)\frac{\pi}{\beta}$ and bosonic Matsubara frequencies with $\omega_n = 2n\frac{\pi}{\beta}$, where $\beta = \frac{1}{T}$ is the inverse temperature and $n \in \mathbb{Z}$. Finally we indicate Matsubara sums as well as integrals over the Brillouin zone as $\sum_\nu := \frac{1}{\beta} \sum_\nu$ and $\sum_k := \frac{1}{V_{\text{BZ}}} \int_{V_{\text{BZ}}} d\mathbf{k}$, respectively.

Ladder DGA

Since the Hubbard model in Eq. (1) is not exactly solvable for the three-, four-, and five-dimensional lattices considered

here, we have to resort to approximate approaches. In a first step, we will exploit DMFT to calculate one- and two-particle correlation functions, in order to capture all purely local correlations of the system. Within this approach, the single-particle Green's function $G_{\mathbf{k}}^\nu$ is obtained as

$$G_{\mathbf{k}}^\nu = \frac{1}{i\nu + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\text{imp}}^\nu}, \quad (3)$$

where Σ_{imp}^ν is the local single particle self-energy of an auxiliary single-impurity Anderson model (SIAM) and μ denotes the chemical potential which fixes the electron density of the system. For the bipartite 3d-sc, bcc, 4d-sc, and 5d-sc lattices, we consider $\mu = \frac{U}{2}$ which enforces half filling $n = 1$, while for the strongly frustrated fcc lattice μ has to be determined to obtain the required filling. The SIAM from which the local self-energy is obtained has to fulfill the following self-consistency condition:

$$\sum_{\mathbf{k}} \frac{1}{\underbrace{i\nu + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\text{imp}}^\nu}_{G_{\mathbf{k}}^\nu}} \stackrel{!}{=} \frac{1}{\underbrace{i\nu + \mu - \Delta_{\text{imp}}^\nu - \Sigma_{\text{imp}}^\nu}_{G_{\text{imp}}^\nu}}, \quad (4)$$

where Δ_{imp}^ν is the hybridization function which defines the SIAM and $G_{\text{imp}}^\nu = [i\nu + \mu - \Delta_{\text{imp}}^\nu - \Sigma_{\text{imp}}^\nu]^{-1}$ represent the local impurity Green's function.

The DMFT spin (magnetic) susceptibility $\chi_{m,\mathbf{q}}^\omega$ is obtained by summing the generalized susceptibility over the fermionic Matsubara frequencies

$$\chi_{m,\mathbf{q}}^\omega = \sum_{\nu\nu'} \chi_{m,\mathbf{q}}^{\nu\nu'\omega}, \quad (5)$$

where $\chi_{m,\mathbf{q}}^{\nu\nu'\omega}$ can be calculated from the DMFT Green's function $G_{\mathbf{k}}^\nu$ in Eq. (3) and the local irreducible spin vertex $\Gamma_m^{\nu\nu'\omega}$ via the Bethe-Salpeter (BS) equation

$$\chi_{m,\mathbf{q}}^{\nu\nu'\omega} = \chi_{0,\mathbf{q}}^{\nu\nu'\omega} - \sum_{\nu_1\nu_2} \chi_{0,\mathbf{q}}^{\nu\nu_1\omega} \Gamma_m^{\nu_1\nu_2\omega} \chi_{m,\mathbf{q}}^{\nu_2\nu'\omega}, \quad (6)$$

where $\chi_{0,\mathbf{q}}^{\nu\nu'\omega} = -\beta \sum_{\mathbf{k}} G_{\mathbf{k}}^{\nu+\omega} G_{\mathbf{k}+\mathbf{q}}^{\nu'} \delta_{\nu\nu'}$ is the so-called bubble contribution to the susceptibility which does not include vertex corrections.

As a mean-field theory with respect to spatial degrees of freedom DMFT typically overestimates ordered states which is reflected in an overestimation of the corresponding spin susceptibility $\chi_{m,\mathbf{q}}^\omega$. This problem can be mitigated by taking into account the contribution of nonlocal correlations within the DGA. Within this approach the mutual renormalization between nonlocal fluctuations in the charge-, spin-, and particle-particle scattering channels are taken into account by means of the parquet equations [37,55–61], which construct all one- and two-particle correlation functions and susceptibilities from a single input, i.e., the fully irreducible two-particle vertex $\Lambda_{\text{imp},\sigma\sigma'}^{\nu\nu'\omega}$ of the auxiliary SIAM. Note that the frequency dependence of this vertex function directly encodes the highly nonperturbative [62] physics of electronic localization [63–66] associated with the Mott transition as well as strong quasiparticle renormalization effects. While this procedure would certainly provide the most accurate results, it is limited to rather high temperatures above the

transition to magnetically ordered phases due to its considerable numerical complexity and, hence, not suitable for the present study. We, therefore, stick to the ladder approximation of D Γ A (ID Γ A) where $\chi_{m,\mathbf{q}}^\omega$ is evaluated via Eqs. (5) and (6) which requires only a solution of a single BS equation in one channel. On the down side, this procedure leads to a violation of an exact sum rule (which would be instead automatically fulfilled within the parquet technique) given by

$$\frac{1}{2} \sum_{\omega\mathbf{q}} (\chi_{d,\mathbf{q}}^\omega + \chi_{m,\mathbf{q}}^\omega) \stackrel{!}{=} \frac{n}{2} \left(1 - \frac{n}{2}\right), \quad (7)$$

where $\chi_{d,\mathbf{q}}^\omega$ is the charge susceptibility which can be obtained in a completely analogous way as the corresponding spin susceptibility in Eqs. (5) and (6). To restore this sum rule within our ladder approach we apply an effective correction to the DMFT spin susceptibility via a constant parameter λ which transforms the DMFT to the ID Γ A spin susceptibility

$$\chi_{m,\mathbf{q}}^{\lambda,\omega} = \frac{1}{(\chi_{m,\mathbf{q}}^\omega)^{-1} + \lambda}. \quad (8)$$

This idea has been first suggested by Moriya in his work on itinerant magnetism [67] and later exploited in the ladder D Γ A [39]. The value of λ is determined to satisfy the sum rule in Eq. (7). This λ correction has a clear physical interpretation: Close to a phase transition the static ($\omega = 0$) spin susceptibility takes an Ornstein-Zernike [68] form

$$\chi_{m,\mathbf{q}}^{\omega=0} = \frac{A}{(\mathbf{q} - \mathbf{q}_N)^2 + \xi^{-2}}, \quad (9)$$

where $\mathbf{q}_N$ is the ordering vector (equivalent to the nesting vector in bipartite lattices), ξ is the correlation length and A is a (temperature dependent) parameter. Within this picture, the λ correction corresponds to a simple renormalization of the correlation length, which is overestimated within DMFT and reduced by the effective inclusion of nonlocal correlations and mutual renormalization via the λ parameter.

III. NUMERICAL RESULTS

In the following, we discuss our numerical results for the five lattices under consideration. The 3d-sc, bcc, 4d-sc, and 5d-sc lattices are bipartite, which implies their perfect particle-hole symmetry at half filling ($n = 1$ particle per lattice site.) In this situation, the Fermi surface is independent of the interaction strength U as well as of the temperature T , and features perfect nesting, i.e., for each point $\mathbf{k}$ on the Fermi surface $\mathbf{k} + \mathbf{q}_N$ is also located on the Fermi surface where $\mathbf{q}_N$ is the so-called nesting vector. The latter property entails a strong tendency to magnetic order at wave vector $\mathbf{q}_N$ indicated by a large (static) spin-susceptibilities $\chi_{m,\mathbf{q}_N}^{\omega=0}$. As we are particularly interested in the corresponding large spin fluctuations above the transition temperature to the ordered state as a function of the interaction strength U , we will perform our analysis exactly at half filling.

The fcc lattice, on the other hand, is strongly geometrically frustrated which leads to a substantial suppression of magnetic order. This has been indeed observed in real materials with a fcc lattice structure such as $\text{Ba}_2\text{LnSbO}_6$ and $\text{Sr}_2\text{LnSbO}_6$ double perovskites (with $\text{Ln} = \text{Dy}, \text{Ho}, \text{Gd}$) where no

magnetic order is found down to $T = 2$ K [69], in the molecular antiferromagnet fcc- Cs_3C_{60} where $T_N = 2.2$ K [70], and in $\text{Ba}_2\text{YbTaO}_6$ where no magnetic long-range order is found down to $T = 100$ mK [71]. Let us, however, note that a next-nearest neighbor hopping in the fcc lattice, which favors a type-II antiferromagnetic order where ferromagnetic layers are antiferromagnetically stacked along the [111] direction and spins at neighboring corners of the cube are pointing in opposite direction, can again enhance magnetic order as it is for instance the case in NiO [72]. On the theoretical side, the suppression of antiferromagnetic order is associated with the absence of particle-hole symmetry where even at half filling no nesting vector exists which would enhance spin fluctuations. In fact, at exactly $n = 1$ RPA and slave boson methods [73] predict that the system is at the verge of a number of competing magnetic phases (including also regions of phase separation) at $T = 0$ which makes our numerical analysis challenging also at finite temperatures (see the RPA analysis in Appendix). Hence, for studying the magnetic transition of the fcc lattice, we have selected $n = 0.75$ around which a stable ordered ground state with the ordering vector $\mathbf{q}_N = (0, 0, 2\pi)$ is observed in RPA (see the Appendix). However, since the strong geometric frustration makes the fcc lattice rather different from the four others, we will discuss the latter together and address the fcc lattice in a separate paragraph for each observable/correlation function which we present in the following.

A. Frequency and momentum dependence of spin susceptibilities

In this section, we analyze the frequency and momentum dependence of the spin susceptibilities for different temperatures and interaction strengths for both the bipartite and the fcc lattices.

Bipartite lattices. In Fig. 2, the spin susceptibilities $\chi_{m,\mathbf{q}=\mathbf{q}_N}^\omega$ at the nesting vector $\mathbf{q} = \mathbf{q}_N$ (see caption of Fig. 2) are compared between DMFT (blue crosses) and ID Γ A (orange circles) as a function of the bosonic Matsubara frequency ω for the 3d-sc, bcc, 4d-sc, and 5d-sc lattices in the first, second, third, and fourth row, respectively, at $\beta = 5.0$ (left panels), $\beta = 10.0$ (middle panels) and $\beta = 12.0$ (right panels) for $U = 2.0$. Let us note, that at the nesting (ordering) vector $\mathbf{q} = \mathbf{q}_N$ the largest difference between DMFT and ID Γ A is expected. The spin susceptibilities are always strongly peaked at $\omega = 0$ as classical spin fluctuations are typically predominant. At the largest temperature $\beta = 5.0$ (left panels in Fig. 2), our D Γ A results almost coincide with the DMFT data, which is consistent with the fact that DMFT becomes the exact solution of the Hubbard model also in the limit of infinite temperatures (where the system becomes effectively noninteracting as the energy scale of the interaction becomes negligible compared to the temperature). Upon decreasing the temperature and approaching the DMFT phase transition to the magnetically ordered state, we observe that both DMFT and D Γ A spin susceptibilities are enhanced, whereas the DMFT one increases much faster (middle panels). This difference between DMFT and D Γ A data is a consequence of the renormalization of $\chi_{m,\mathbf{q}}^\omega$ within the ID Γ A to fulfill the sum rule in Eq. (7). At the lowest temperatures (right panels) DMFT already predicts

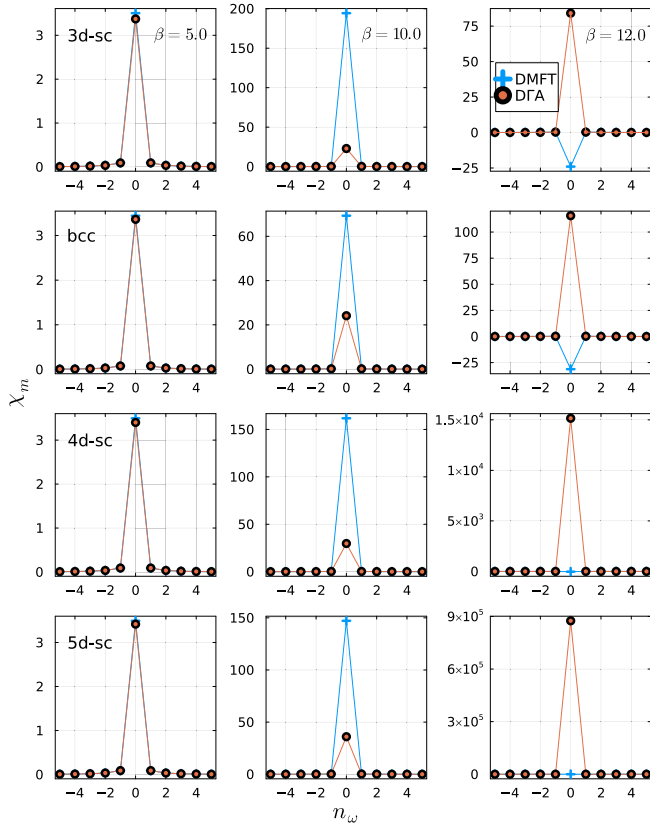


FIG. 2. Spin susceptibilities $\chi_{m,\mathbf{q}=\mathbf{q}_N}^\omega$ at $U = 2.0$ and $n = 1.0$ for the three temperatures $\beta = 5.0$ (left panels), $\beta = 10.0$ (middle panels) and $\beta = 12.0$ (right panels) for the 3d-sc (first row), bcc (second row), 4d-sc (third row), and 5d-sc (fourth row) lattices, respectively. Data are shown for DMFT (blue crosses) and IDΓA (orange circles). The nesting vectors (which correspond to antiferromagnetic ordering vectors for bipartite lattices) are $\mathbf{q}_N = (\pi, \pi, \pi)$ (3d-sc), $\mathbf{q}_N = (2\pi, 2\pi, 2\pi)$ (bcc), $\mathbf{q}_N = (\pi, \pi, \pi, \pi)$ (4d-sc), and $\mathbf{q}_N = (\pi, \pi, \pi, \pi, \pi)$ (5d-sc).

an ordered phase indicated by the negative spin susceptibility at $\omega = 0$ which is turned to a large but positive value via the λ correction within DΓA for which, instead, we are still in the paramagnetic regime. Note that the absolute values of $\chi_{m,\mathbf{q}=\mathbf{q}_N}^\omega$ are quite different between the four lattice types, due to the difference in their respective DMFT and DΓA transition temperatures.

In Fig. 3 we depict the static spin susceptibility $\chi_{m,\mathbf{q}}^{\omega=0}$ as function of the momentum $\mathbf{q}$ along a high-symmetry path in the Brillouin zone for $U = 2.0$ for the 3d-sc, bcc, 4d-sc, and 5d-sc lattices, respectively. We present only DMFT data here as the functional form of $\chi_{m,\mathbf{q}}^{\omega=0}$ cannot be modified by the momentum independent λ correction of IDΓA and the overall reduction in size due to this correction has already been discussed for the local spin susceptibilities in Fig. 2. Even for the rather high temperature $\beta = 5.0$, we observe a clear peak of these correlation functions at the respective ordering (nesting) vector $\mathbf{q}_N$ for all four bipartite lattices. This demonstrates that spin fluctuations are strongly pronounced already quite far away from the low-temperature phase transition.

fcc lattice. The results for the frequency and momentum dependence of the spin susceptibility for the fcc lattice are

presented in Figs. 4 and 5, respectively. At high temperatures (inset in the left panel of Fig. 4), the peak in the local spin susceptibility $\chi_{m,\text{loc}}^\omega$ at $\omega = 0$ is considerably reduced compared to the bipartite lattices in the left panels of Fig. 2. This indicates a strong suppression of magnetic fluctuations which is consistent with the geometric frustration and the absence of nesting in the fcc lattice. The peak at $\omega = 0$ can be, however, increased by substantially lowering the temperature beyond the ones considered for the 3d-sc, bcc, 4d-sc, and 5d-sc in Fig. 2. At $\beta = 20.0$ (left panel of Fig. 4) we observe a moderate value of the local spin susceptibility at $\omega = 0$ which is roughly equivalent for DMFT and DΓA indicating that non-local correlations are rather insignificant at this temperature. On the contrary, at $\beta = 150$ (right panel) we see a pronounced difference between DMFT and DΓA albeit no phase transition is observed at such low temperature even in DMFT, in strong contrast to the bipartite lattices.

The static spin susceptibility $\chi_{m,\mathbf{q}}^{\omega=0}$ at high temperatures (not shown), on the other hand, is rather flat as a function of $\mathbf{q}$ at $n = 1.0$ without any pronounced features at a specific wave vector. This is again a consequence of the strong geometric frustration in the lattice. Hence, in Fig. 5, we present data for $\chi_{m,\mathbf{q}}^{\omega=0}$ of the fcc lattice for $n = 0.75$ where at a rather low temperature of $\beta = 80.0$ this correlation function features a clear peak at $\mathbf{q} = \mathbf{q}_N = (0, 0, 2\pi)$ indicating a tendency to a magnetic ordering at this momentum vector. We note that such an ordering vector corresponds to a layered antiferromagnetic pattern where planes with spin up and spin down perpendicular to the q_z direction alternate. This is consistent with predictions from RPA and slave-boson studies [73] for the ground state at $n = 0.75$ (see also, the Appendix).

B. Temperature dependence of the spin susceptibility

In this section, we analyze the temperature dependence of the static ($\omega = 0$) spin susceptibility at the ordering vector $\mathbf{q}_N$ (which is equivalent to the nesting vector for the bipartite case) for selected interaction strengths. For convenience, we will denote this quantity as antiferromagnetic susceptibility $\chi_{\text{AF}}(T) = \chi_{m,\mathbf{q}=\mathbf{q}_N}^{\omega=0}(T)$, also for the fcc lattice where the geometric structure of the order does not correspond to a textbook G-type antiferromagnet due to geometric frustration. Close to the transition temperature to the magnetically ordered state $\chi_{\text{AF}}(T)$ follows the universal scaling law:

$$\chi_{\text{AF}}(T) = \chi_{m,\mathbf{q}=\mathbf{q}_N}^{\omega=0}(T) \sim A(T - T_N)^{-\gamma}, \quad (10)$$

where A is a constant, T_N the transition temperature to the ordered state, and γ the critical exponent associated with a second-order phase transition. The functional form in Eq. (10) implies that the susceptibility features a power law divergence at $T = T_N$. We present our results for the bipartite and the fcc lattices in the two following separate paragraphs.

Bipartite lattices. In Fig. 6 we show our data for the inverse antiferromagnetic spin susceptibility $\chi_{\text{AF}}^{-1}(T)$ as function of temperature T for the bipartite 3d-sc, bcc, 4d-sc, and 5d-sc lattices. Blue circles correspond to DMFT results, while our IDΓA data are represented by orange triangles. The temperature at which $\chi_{\text{AF}}^{-1}(T)$ crosses zero corresponds to the transition temperature T_N to the magnetically ordered state. Within DMFT $\chi_{\text{AF}}^{-1}(T)$ is a straight line for all bipartite

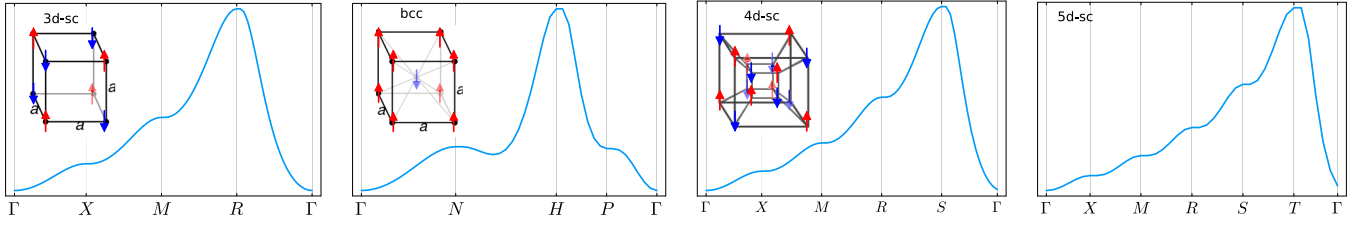


FIG. 3. Momentum dependence of the static DMFT susceptibilities $\chi_{m,q}^{\omega=0}$ along a high-symmetry path for the 3d-sc (first panel), the bcc (second panel), the 4d-sc (third panel), and the 5d-sc (fourth panel) lattice, respectively, at $U = 2.0$, $n = 1.0$ and $\beta = 5.0$. Since there is no established convention for labeling high symmetry points in the 4d-sc and 5d-sc lattice, we choose a notation similar to the 3d-sc lattice: $\Gamma = (0, 0, 0, 0)$, $X = (0, 0, 0, \pi)$, $M = (0, 0, \pi, \pi)$, $R = (0, \pi, \pi, \pi)$, $S = (\pi, \pi, \pi, \pi)$ for the 4d-sc lattice and $\Gamma = (0, 0, 0, 0, 0)$, $X = (0, 0, 0, 0, \pi)$, $M = (0, 0, 0, \pi, \pi)$, $R = (0, 0, \pi, \pi, \pi)$, $S = (0, \pi, \pi, \pi, \pi)$ and $T = (\pi, \pi, \pi, \pi, \pi)$ for the 5d-sc lattice. Insets: geometrical structure of the lattices replotted from Fig. 1 where the arrows represent the predominant spin order.

lattices which is consistent with the standard mean-field critical exponent $\gamma = 1$. The nonlocal correlations included by D Γ A affect the antiferromagnetic susceptibility in two ways: (i) As expected, at high temperatures our ID Γ A data almost coincide with the DMFT results for $\chi_{AF}^{-1}(T)$. As T decreases the ID Γ A data for $\chi_{AF}^{-1}(T)$ start to deviate from the DMFT results while still keeping a linear dependence on T albeit with a reduced slope. Already this deviation from DMFT leads to a zero-crossing of the ID Γ A $\chi_{AF}^{-1}(T)$ at lower temperatures than in DMFT, hence, featuring a reduced critical temperature. For the 3d-sc and the bcc lattices (upper left and right panel, respectively) this reduction of T_N gets further enhanced by (ii) a deviation from the linear shape at low temperature close to the phase transition, where the critical exponent γ becomes visually larger than one. The temperature region $\Delta T_{\text{crit}} = T - T_N$ where such a deviation from the linear behavior can be observed can be estimated via the Ginzburg-Landau criterion [74] which yields $\Delta T_{\text{crit}} \propto T_N^2$. Let us note, however, that the critical region is smaller for the bcc with respect to the 3d-sc lattice which is consistent with the fact that the bcc lattice has a larger coordination number and, hence, DMFT may be expected to be more accurate for this system in a broader parameter regime. For the 4d-sc in the lower left panel of Fig. 6 our numerical ID Γ A data indicate that $\gamma = 1$ coinciding with the mean-field prediction. This is indeed the expected behavior in four dimensions although logarithmic corrections can be expected as $d = 4$ corresponds to the upper critical dimensions. These logarithmic corrections can make the numerical fitting procedure more challenging which we will discuss below in more detail. In any case, the sizable reduction of T_N observed for the 4d-sc lattice originates exclusively from

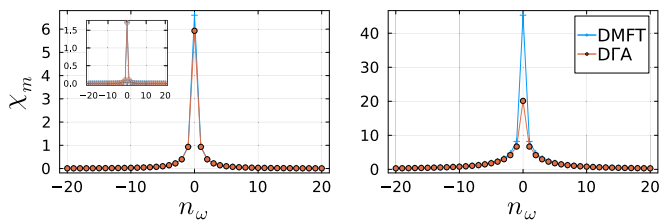


FIG. 4. Spin susceptibility $\chi_{m,q}^{\omega}$ for the fcc lattice at $U = 3.0$ and $n = 0.75$ for $\beta = 5.0$ (inset of left panel), $\beta = 20.0$ (left panel), and $\beta = 150.0$ (right panel). The ordering vector $\mathbf{q}_N = (0, 0, 2\pi)$ corresponds to the layered antiferromagnetic order depicted in Fig. 5.

feature (i), i.e., the rigid shift of $\chi_{AF}^{-1}(T)$ by ID Γ A discussed above. Finally, for the 5d-sc lattice a deviation from the linear temperature dependence of $\chi_{AF}^{-1}(T)$ predicted by DMFT is *not* observed in our ID Γ A data (lower right panel of Fig. 6), thus yielding $\gamma \sim 1$. This is fully consistent with the general understanding that for $d \geq 5$ mean-field critical behavior is recovered as the exact solution of the problem.

In a next step, we have analyzed the temperature dependence of $\chi_{AF}^{-1}(T)$ close to T_N more accurately for the 3d-sc and the bcc lattices, where evident deviations from the mean-field exponent are observed. This has allowed us to investigate the critical behavior more thoroughly and, in particular, to provide accurate estimates for the critical temperature T_N and the critical exponent γ in Eq. (10). To this end, we have fitted our numerical data for $\chi_{AF}^{-1}(T)$ to Eq. (10). The results of these fits, which are shown as orange lines in the insets of the upper panels of Fig. 6 for the 3d-sc and bcc lattice, respectively, as well as for the 3d-sc on a larger scale in the left panel (a) of Fig. 7, predict a critical exponent of $\gamma = 1.556$ for the bcc and $\gamma = 1.7026$ for the 3d-sc lattice. The latter value for the 3d-sc lattice is in good agreement with previous ladder D Γ A [32] and dual fermion [45] calculations for this lattice.

Let us, however, note that the actual critical exponent can be precisely observed only extremely close to the phase

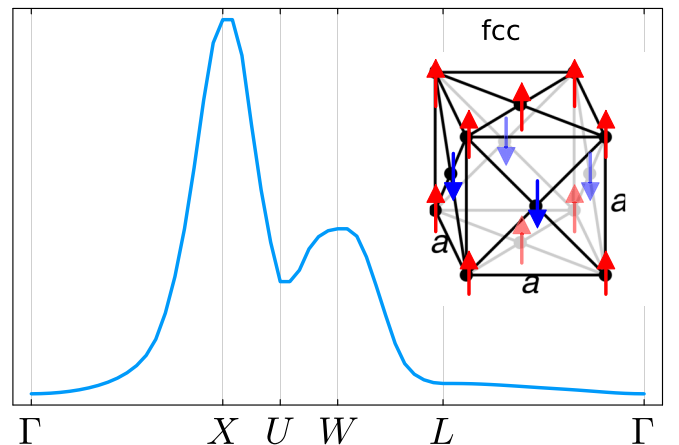


FIG. 5. Momentum dependence of the static DMFT susceptibilities $\chi_{m,q}^{\omega=0}$ along a high-symmetry path for the fcc lattice at $U = 3.0$, $n = 0.75$, and $\beta = 80.0$. The spin-ordered state represented by the arrows corresponds to the ordering vector $\mathbf{q} = (0, 0, 2\pi)$.

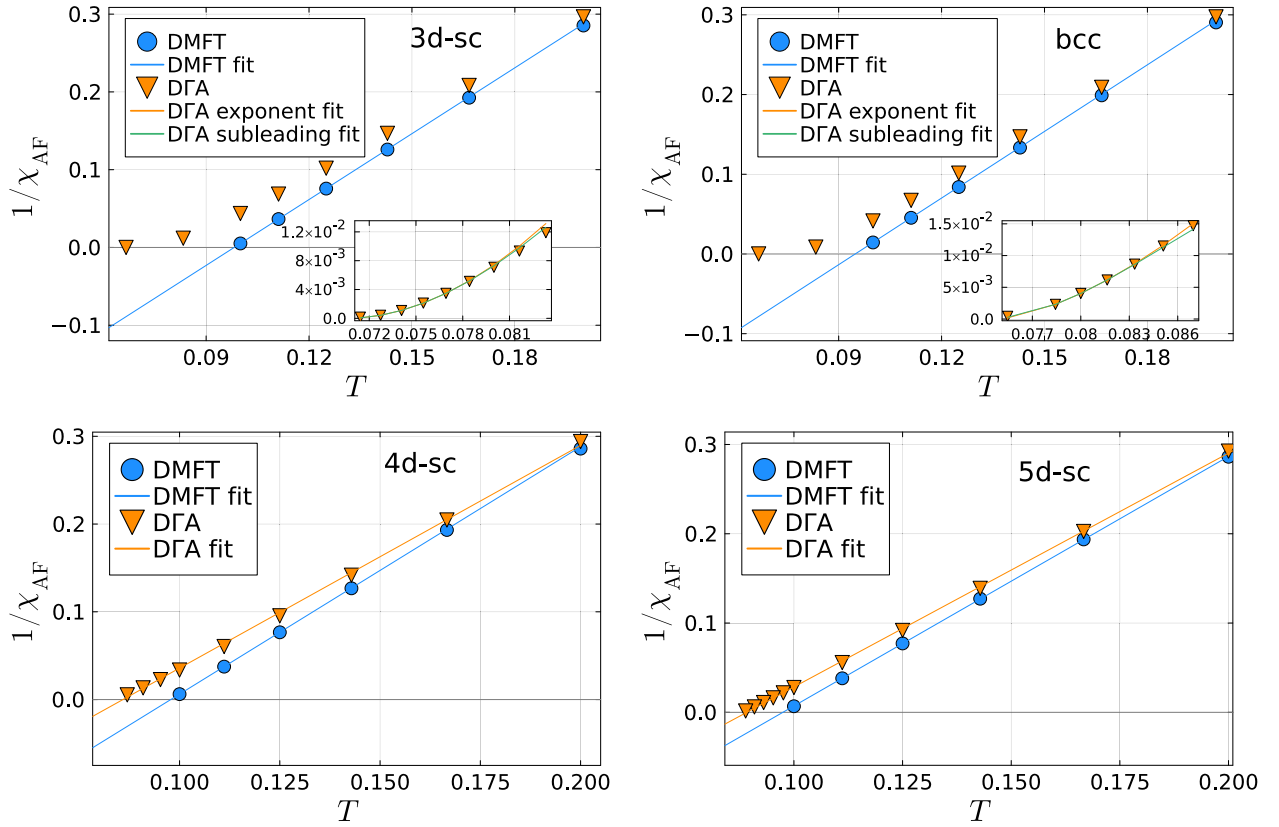


FIG. 6. Inverse antiferromagnetic susceptibility $1/\chi_{\text{AF}}(T) = 1/\chi_{m,q=\mathbf{q}_N}^{\omega=0}(T)$ as function of the temperature T at $U = 2.0$ for the 3d-sc [$\mathbf{q}_N = (\pi, \pi, \pi)$, top left panel], bcc [$\mathbf{q}_N = (2\pi, 2\pi, 2\pi)$, top right panel], 4d-sc [$\mathbf{q}_N = (\pi, \pi, \pi, \pi)$, bottom left panel], and 5d-sc [$\mathbf{q}_N = (\pi, \pi, \pi, \pi, \pi)$, bottom right panel] lattice, respectively. DMFT and DfA results are indicated by blue circles and orange triangles. Blue lines represent linear fits to the DMFT data. For the 3d-sc and the bcc lattices, the inset shows fits to the numerical IDfA data for the two fitting functions in Eqs. (10) and (11). For the 4d-sc and 5d-sc lattices the orange line is a linear fit to the IDfA data.

transition, while at larger values of T deviations from the scaling behavior in Eq. (10) emerge. Fitting our numerical results, which due to the accessible range partly include such data at higher temperatures, to this scaling function will then result in an inaccurate determination of the critical exponent γ . To mitigate this problem and obtain more reliable results we have, hence, devised the following procedure illustrated in Fig. 7(b), which allows us to gradually improve the accuracy

of the numerical value for γ : We start at rather high temperatures far away from T_N by fitting the numerical data for $\chi_{\text{AF}}^{-1}(T)$ to Eq. (10) using only three data points corresponding to the temperatures T_1, T_2 and T_3 which are indicated by green circles in Fig. 7(b). We denote the obtained value of γ as $\gamma(T_3)$ since T_3 is the last point of this data set. In the next step, we replace the data point at the highest temperature T_1 with the data point at T_4 which is one step lower than

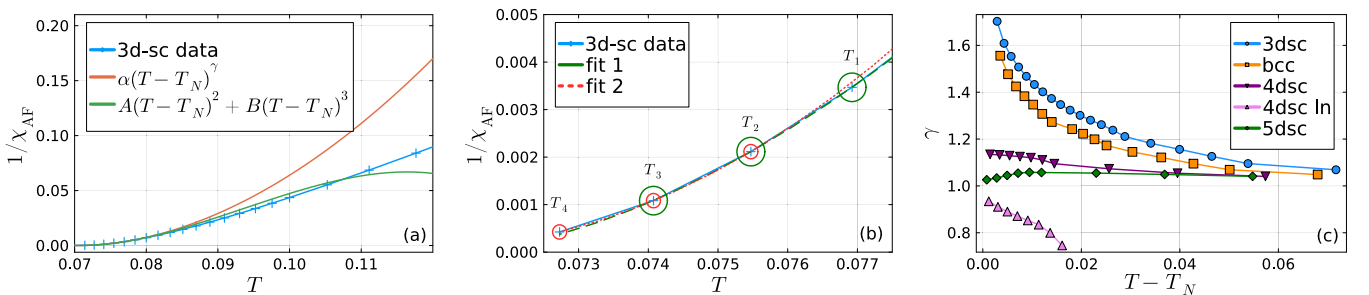


FIG. 7. (a) Numerical IDfA data for $\chi_{\text{AF}}^{-1}(T)$ for the 3d-sc lattice at $U = 2.0$ (blue crosses) fitted to Eqs. (10) (orange line) and (11) (green line). (b) Illustration of the fitting procedure (for the 3d-sc lattice) used to obtain the critical exponent γ in Eq. (10) where only three data points are used for the fit indicated by large green and small red circles which gradually approach T_N . (c) Fitted value of the critical exponent γ as a function of the distance from $T - T_N$ where the fit has been performed according to the procedure outlined in the (b). Data in the (b) and (c) correspond to $U = 2.0$. For the 4d-sc we present data from fits without (violet lower triangles) and with (pink upper triangles) logarithmic corrections.

the lowest previous data point at T_3 . Hence, the new data set which we use for the next fit consists of the values for $\chi_{\text{AF}}^{-1}(T)$ at the temperatures T_2 , T_3 and T_4 [indicated by red circles in Fig. 7(b)] and gives us a new critical exponent $\gamma(T_4)$. Iterating this procedure we obtain a function $\gamma(T = T_i)$ where T_i always corresponds to the lowest of the three temperatures. We have plotted this function $\gamma(T)$ relative to T_N in Fig. 7(c) for the 3d-sc (blue circles), bcc (orange squares), 4d-sc (violet lower and pink upper triangles), and 5d-sc (green diamonds) lattices. For the 3d-sc and bcc lattices we clearly see that $\gamma(T)$ has not saturated at the smallest temperatures but, on the contrary, is very steep which indicates that a larger critical exponent γ than the previously fitted values of $\gamma = 1.7026$ for the 3d-sc and $\gamma = 1.556$ for the bcc lattice can be expected. In fact, a fit of the curve $\gamma(T)$ to $T \rightarrow T_N$ predicts values of $\gamma \sim 1.89$ for the 3d-sc lattice and $\gamma \sim 1.76$ for the bcc lattice. It seems likely that these values might further increase if we could evaluate $\chi_{\text{AF}}^{-1}(T)$ for temperatures even closer to T_N (which is numerically infeasible).

The above considerations have motivated us to consider the question of the critical exponent γ for the 3d-sc and the bcc lattice obtained within ID Γ A from a more general perspective. Indeed, it was numerically observed in Ref. [75], where ID Γ A calculations were performed for the attractive Hubbard model on a 3d-sc lattice, that the fitted exponents appeared compatible with the universality class of the Berlin-Kac model where the number of components of the order parameter $N \rightarrow \infty$ (corresponding to a mean field in the dimension of the order parameter), similar as those of the two-particle-self-consistent approach [76]. In fact, the value of $\gamma = 2$ associated to the Berlin-Kac universality class [76] appears well compatible also with our numerical data, when we fix $\gamma = 2$ and include a subleading term proportional to $(T - T_N)^3$ in our numerical fit function

$$\chi_{\text{AF}}^{-1}(T) = A(T - T_N)^2 + B(T - T_N)^3. \quad (11)$$

We have tested this fit function for the 3d-sc and the bcc lattice in the insets of the upper panels of Fig. 6 and Fig. 7(a) (green curve), finding an excellent agreement with our numerical data. This indicates that, in three dimensions, ID Γ A calculations with infinite numerical precision (not feasible in practice) might indeed yield the value of $\gamma = 2$ of the Berlin-Kac model, thus overestimating the expected exact value for the 3d-Heisenberg universality class ($\gamma \simeq 1.41$).

For the 4d-sc, we expect a critical exponent $\gamma = 1$ (with logarithmic corrections) as we are at the upper critical dimension. Our numerical data for $\gamma(T)$ for the 4d-sc lattice in Fig. 7(c) indeed shows only a weak dependence of $\gamma(T)$ on T , which varies between 1.0 and 1.15. To better understand the small deviation from the expected value of $\gamma = 1$ we have made a second fit using a fit function which includes the logarithmic corrections [77]

$$\chi_{\text{AF}}(T) = \chi_{m, \mathbf{q}=\mathbf{q}_N}^{\omega=0}(T) \sim A(T - T_N)^{-\gamma} \ln \left(\frac{1}{T - T_N} \right)^{\hat{\gamma}}, \quad (12)$$

where we have set $\hat{\gamma} = 1$ which corresponds to the value expected for the Berlin-Kac model. With this ansatz our values for γ become smaller than 1 [upper pink triangles in Fig. 7(c)] and rapidly approach the expected value of 1 from below.

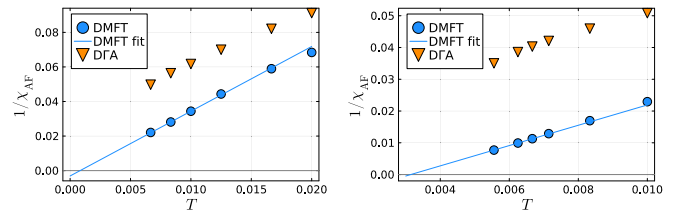


FIG. 8. Inverse antiferromagnetic susceptibility $1/\chi_{\text{AF}}(T) = 1/\chi_{m, \mathbf{q}=\mathbf{q}_N}^{\omega=0}(T)$ for $\mathbf{q}_N = (0, 0, 2\pi)$ as a function of T for the fcc lattice at $U = 3.0$ (left panel) and $U = 5.0$ (right panel) for $n = 0.75$. The blue line is a linear fit to the DMFT data.

Hence, although the fitting procedure is numerically delicate in 4d we conclude that our numerical data are compatible with the expected value $\gamma = 1$ when logarithmic corrections are included in the fit function.

Finally, for the 5d-sc lattice [green diamonds in Fig. 7(c)] we observe a very good agreement with the expected mean-field critical exponent $\gamma = 1$ close to the phase transition. The very small deviations can be attributed to the finite numerical precision and the numerical limitations for the size of the momentum grids in 5d.

fcc lattice. The results for $\chi_{\text{AF}}^{-1}(T)$ in the fcc lattice are depicted in Fig. 8 for the two different interaction strengths $U = 3.0$ (left panel) and $U = 5.0$ (right panel) at $n = 0.75$. As already discussed in the previous section, spin fluctuations are strongly suppressed in this lattice due to the large geometric frustration. In order to observe an appreciable antiferromagnetic susceptibility, we have to consider very low temperatures and large interaction strengths where numerical calculations are notoriously difficult. Within DMFT (blue circles) we find the expected linear behavior of $\chi_{\text{AF}}^{-1}(T)$ for both considered interaction strengths. We can see that for $U = 3.0$ in the left panel $T_N \simeq 0$ which indicates that no magnetic order can be observed in the fcc lattice for $U \lesssim 3.0$. Hence, while in the bipartite lattices a magnetic order is observed for all interaction strengths both in DMFT and DfA such an order emerges in the fcc lattice only above a critical interaction strength $U_c \approx 3.0$ in DMFT.

Remarkably, the inclusion of nonlocal correlations obtained via ID Γ A (orange triangles) *completely* suppresses the antiferromagnetic order predicted by DMFT, as no zero-crossing of $\chi_{\text{AF}}^{-1}(T)$ can be anticipated from the extrapolation of this correlation function to small temperatures. It appears that the DfA results are also linear in T , which would be consistent with the large coordination number of 12 for the fcc lattice where a mean-field exponent can be expected in a broad region of the phase diagram. Let us, however, mention that the determination of λ at very low temperatures is numerically extremely challenging, which limits the conclusions we can draw on the $T \rightarrow 0$ magnetic properties in the fcc lattice.

C. Phase diagram

In this section, we determine the transition curve $T_N(U)$ by extracting the values of T_N at which $\chi_{\text{AF}}^{-1}(T)$ crosses zero for a range of interaction values U . The results are reported in Fig. 9 where solid lines represent the DfA data and dashed lines correspond to the DMFT results. In the main panel the

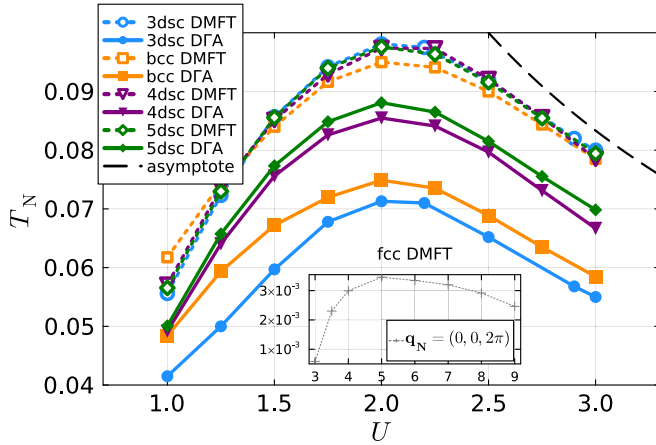


FIG. 9. Phase diagram for the 3d-sc (blue circles), bcc (orange squares), 4d-sc (violet triangles), and 5d-sc (green diamonds) lattices obtained from DMFT (empty symbols/dashed lines) and IDΓA (filled symbols/solid lines). The inset shows the (approximate) $T_N(U)$ obtained by DMFT for the fcc lattice.

IDΓA Néel temperatures for the bipartite lattices are shown, while the fcc transition temperature is presented in the inset (for DMFT only).

Bipartite lattices. For the four bipartite lattices we observe a sizable reduction of T_N of DMFT (empty symbols/dashed lines) by nonlocal correlations computed in IDΓA (filled symbols/solid lines). The size of the reduction depends on the dimension and the coordination number of the lattice. In fact, while we have chosen our system parameters in such a way that the transition temperatures in DMFT are (almost) equivalent for all bipartite lattices, the associated IDΓA curves are visibly different. The largest deviation for T_N between DMFT and IDΓA is observed for the 3d-sc lattice (blue empty and filled circles) which has a coordination number of 6. For the bcc lattice (orange empty and filled squares) with a coordination number of 8, this difference is already smaller with respect to the 3d-sc lattice case, consistent with higher accuracy of DMFT for larger coordination numbers. An even smaller difference for T_N between DMFT and IDΓA is observed for the tesseract lattice, which has the same coordination number 8 as the bcc one but lives in four spatial dimensions. Here, the mean-field critical exponent $\gamma = 1$ prevents a further reduction of T_N in the critical region compared to the bcc case for which $\gamma > 1$. As expected, the 5d-sc lattice exhibits the smallest deviation between DMFT and IDΓA since it has the highest coordination number ($Z = 10$). Let us point out, that while the gap between the IDΓA phase transition for the 3d-sc and 4d-sc is rather large the difference in T_N between the 4d-sc and 5d-sc lattice is substantially smaller. This might originate from the difference in the critical exponent γ between three and four dimensions (while they are equivalent for four and five dimensions) and indicates a rather slow convergence to the $d = \infty$ limit where T_N of IDΓA should become equivalent to the corresponding DMFT value. To better quantify our results, we provide in Table I the relative reduction of T_N between DMFT and IDΓA for all lattice types.

Let us also analyze the asymptotic behavior of T_N for large values of the interaction strength U . In this limit the

TABLE I. Reduction of the DMFT Néel temperature by IDΓA (in percent) at different values of U for the four bipartite lattices under consideration.

U	1.0	1.25	1.5	1.75	2.0	2.25	2.5	2.75	3.0
3d-sc	25.4	30.8	30.3	28.0	27.3	27.2	29.1	30.7	31.2
bcc	21.6	20.2	20.0	21.5	21.2	21.9	23.5	24.7	25.5
4d-sc	13.8	13.0	11.2	11.1	12.2	13.6	13.5	14.6	15.1
5d-sc	11.4	9.9	9.6	9.7	9.7	10.2	11.0	11.6	12.1

(bipartite) Hubbard model can be mapped onto an Heisenberg model $H_{\text{Heis}} = J \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j$ via a Schrieffer-Wolff transform [78] where $J = \frac{4t^2}{U} > 0$ couples two neighboring spins antiferromagnetically. Within DMFT this leads to an Ising type result for T_N (for spin 1/2 particles) which is given by $T_N = \frac{z^2}{U}$ where z is the coordination number of the lattice. Since in this work we have fixed $zt^2 = \frac{1}{4}$ for all lattices the asymptotic behavior of the DMFT transition temperatures coincide between all bipartite lattices taking a value of $T_N \sim \frac{1}{4U}$. On the contrary, DΓA takes into account transverse spin fluctuations and, hence, approaches the exact Heisenberg solution for all (bipartite) lattices which are obviously different for the different lattice types.

fcc lattice. For the fcc lattice we could find an antiferromagnetic phase transition within DMFT only for $U > 3.0$ due to the strong geometric frustration in this lattice (see inset in Fig. 9). This T_N of DMFT is reduced to zero by the nonlocal correlations captured by IDΓA for all interaction strengths considered in this study. In fact, in this lattice a magnetic order at finite temperature as predicted by DMFT is a pure correlation effect as no nesting vector exists in the noninteracting dispersion which would lead to a weak-coupling Slater type magnetism [79–82].

D. Weak coupling

Due to our intentional choice of the hopping parameters discussed in the previous Sec. II, the transition temperatures of DMFT in Fig. 9 are very similar for the four bipartite lattices, with an increasing matching in the strong-coupling limit. For intermediate and especially weak coupling on the other hand small but clearly visible differences can be observed in Fig. 9, in particular between T_N for the 3d-sc (empty blue circles) and the bcc (empty orange squares) lattices. More specifically, at the lowest coupling strength $U = 1.0$ the DMFT transition temperature for the bcc lattice is larger than the one for the 3d-sc lattice. On the contrary, at $U = 2.0$ the situation is reversed with a slightly larger T_N for the 3d-sc with respect to the bcc lattice. To verify our DMFT results at weak coupling, where numerical calculations are indeed difficult due to the low values of T_N , we have carried out a semianalytic weak coupling expansion as proposed in Refs. [83] and [84], which should be consistent with the DMFT results for T_N up to $U \sim 1.0$. Within this approach the simple random phase approximation, where the irreducible vertex in the magnetic channel is replaced by the bare interaction $\Gamma_m^{vv'\omega} = -U$, is extended to second order in U by considering

$$\Gamma_{\text{loc}}^{vv'(\omega=0)} = -U + U^2 \chi_{0,\text{loc}}^{pp,v+v'}, \quad (13)$$

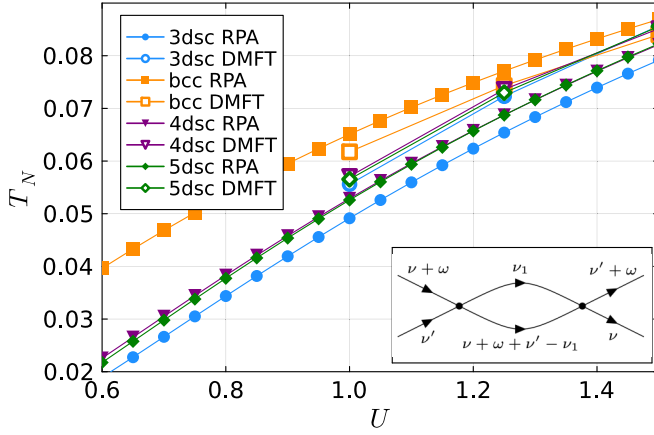


FIG. 10. RPA results for T_N for the 3d-sc (filled blue circles), bcc (filled orange squares), 4d-sc (filled violet triangles) and 5d-sc (filled green diamonds) lattice, which are corrected by the second-order diagrams shown in the inset [see also Eq. (13)]. DMFT results (empty symbols) are given as reference at larger coupling strengths.

where $\chi_{0,\text{loc}}^{pp,v+v'} = \sum_{\nu_1 \mathbf{k}_1 \mathbf{q}} G_0(\nu_1, \mathbf{k}) G_0(\nu_1 + \nu + \nu', \mathbf{k} + \mathbf{q})$ is the bare local pairing susceptibility (particle-particle bubble) and $G_0(\nu, \mathbf{k}) = 1/(i\nu + \mu - \varepsilon_{\mathbf{k}})$ the noninteracting Green's function. At weak-to-intermediate coupling this approximation yields results for T_N as a function of U which are in quite good qualitative agreement with our numerical DMFT calculations. This is demonstrated in Fig. 10 where the second-order results for T_N obtained from Eq. (13) for the 3d-sc (filled blue circles), bcc (filled orange squares), 4d-sc (filled violet triangles), and 5d-sc (filled green diamonds) lattices are reasonably close to the corresponding DMFT data (empty symbols).

More importantly, the approximate calculations also reproduce the correct hierarchy of T_N at weak coupling between the 3d-sc and the bcc lattice as predicted by DMFT. The results of this perturbative approach are mainly determined by the bare (bubble) magnetic susceptibility which is proportional to the noninteracting density of state $D(\varepsilon)$. While for the 3d-sc (and also 4d-sc, 5d-sc) $D(\varepsilon)$ is rather featureless, it exhibits a van Hove singularity at the Fermi level for the bcc lattice. Considering the RPA-like expression for $T_N \sim e^{-1/D(0)}$, which holds also for the approximation in Eq. (13), a higher $D(0)$ as in the bcc lattice implies indeed a higher Néel temperature. At the same time, this higher density of states provides more phase space for electron-electron scattering which increases the correlation effects at larger values of U . These enhanced correlations tend to suppress T_N [30] for the bcc lattice at intermediate coupling strength $U \sim 2.0$ stronger than in the 3d-sc lattice, where such correlation effects are weaker due to the absence of a van Hove singularity. This explains the higher values of T_N for the 3d-sc with respect to the bcc lattice in this parameter regime.

Let us finally mention that the hierarchy of curves in the phase diagram obtained from IDΓA at weak coupling, in particular the equal values of T_N for the bcc and 4d-sc lattices at $U = 1.0$, cannot easily be explained. In this respect we should mention, that the low coupling values for T_N provided by IDΓA with a λ correction only in the spin channel might

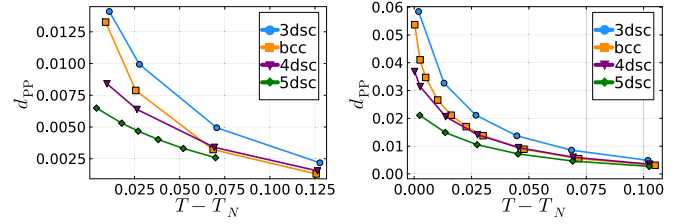


FIG. 11. Violation of the Pauli principle in DMFT [see Eq. (14)] on the 3d-sc (blue circles), bcc (orange squares), 4d-sc (violet triangles), and 5d-sc (green diamonds) lattices at $U = 1.25$ (left panel) and 2.0 (right panel). For $T \rightarrow \infty$ $d_{\text{PP}}(T)$ approaches zero as DMFT becomes exact in this limit.

be underestimated as a renormalization of charge fluctuations is neglected. More accurate results require an improved treatment of charge fluctuations as it has been recently developed for IDΓA in Refs. [85,86].

E. Violation of sum rules

The ladder DΓA includes nonlocal correlation effects in an effective way by restoring the sum rule in Eq. (7), which is violated when using DMFT in finite dimensions. Hence, the magnitude of this violation d_{PP} , which is just the difference between the right- and left-hand side of Eq. (7), can be used as an indicator for the reliability of DMFT results for different lattices and parameter regimes

$$d_{\text{PP}} = \frac{1}{2} \sum_{\omega \mathbf{q}} (\chi_{d,\mathbf{q}}^{\omega} + \chi_{m,\mathbf{q}}^{\omega}) - \frac{n}{2} \left(1 - \frac{n}{2}\right). \quad (14)$$

We have hence calculated d_{PP} for different coupling strengths as a function of T to analyze how the violation of this sum rule depends on the lattice type and the proximity to the antiferromagnetic phase transition. Note that for $T \rightarrow \infty$ this quantity should approach zero as DMFT becomes exact in this limit.

Bipartite lattices. In Fig. 11 we plot the violation d_{PP} of the Pauli principle in Eq. (14) for all bipartite lattices for $U = 1.25$ (left panel) and $U = 2.0$ (right panel), respectively, as a function of $T - T_N$ where T_N denotes the transition temperature of the respective lattice. We clearly observe a pronounced increase of the violation upon approaching the transition temperature of DMFT. This is indeed the expected behavior as the increasingly strong nonlocal fluctuations in the vicinity of the phase transition are not adequately captured in DMFT. The hierarchy between the four bipartite lattices follows their different coordination numbers and spatial dimensions. The largest violation is observed for the 3d-sc lattice with a coordination number of 6 followed by the bcc lattice with a coordination number of 8. Though it has the same coordination number as the bcc lattice, substantially lower increase of d_{PP} in the vicinity of T_N is observed for the tesseract case, due to the additional dimension. Finally, the 5d-sc lattice shows the smallest violation of the Pauli principle at coordination number 10. The evolution of d_{PP} convincingly illustrates the systematically improved quality of DMFT results for higher coordination number and spatial dimensions.

IV. CONCLUSIONS AND OUTLOOK

In this paper we have investigated the impact of nonlocal correlations in strongly correlated electron systems for different lattice geometries. To this end we have considered the Hubbard model for the 3d-sc, bcc, 4d-sc, 5d-sc, and fcc lattices. The first four lattices are bipartite and, hence, feature a strong tendency to antiferromagnetic order, while in the fcc lattice magnetic fluctuations are strongly suppressed due to geometric frustration. In a first step, we have analyzed the transition temperatures T_N to the magnetically ordered state exploiting DMFT, which takes into account local correlations only. In a second step, we have demonstrated how these transition temperatures are reduced by the inclusion of nonlocal correlation effects by means of ID Γ A. We found a clear hierarchy for the differences between DMFT and ID Γ A which decrease with increasing coordination number and dimension of the lattice. This is indeed the expected behavior as DMFT becomes exact in the limit of infinite coordination number or dimension. To complete our analysis of T_N for low values of U we have used a low-coupling expansion of T_N which has allowed us to understand the enhanced value of the transition temperature in the bcc lattice in terms of the van Hove singularity emerging at the Fermi level in this system.

We have also investigated the critical behavior close to T_N and, in particular, calculated the critical exponent γ for all lattice types. While for the 4d-sc and 5d-sc lattices we obtain $\gamma \sim 1$ (except for logarithmic corrections), which is consistent with scaling theory in dimensions $d \geq 4$, our numerical data indicate, (within the specific framework of Moriya corrected ID Γ A) definitely larger values of critical exponents of the three-dimensional bipartite lattices, numerically compatible with the Berlin-Kac model universality class.

Finally, we have quantified the violation of a specific sum rule for the magnetic susceptibilities within DMFT, further supporting the observed hierarchy for the impact of nonlocal correlations for the different lattice geometries according to their coordination number/dimension.

Our work can serve as a useful “compass” for the quantitative description of emerging magnetic orders of correlated electrons in different lattice geometries for both experimental and theoretical studies. Our analysis can be further improved by more sophisticated description of nonlocal correlations which takes into account also charge fluctuations in the weak-to-intermediate coupling regime, which has been recently proposed in Refs. [85] and [86]. Moreover, the study of the fcc lattice could be extended to other fillings where a wide variety of different phases is observed by weak-coupling methods.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX: RPA RESULTS FOR THE FCC LATTICE

The fcc lattice features a strong geometric frustration which leads, in general, to a substantial suppression of magnetically ordered phases. Moreover, the absence of a nesting vector prevents a clearly dominating type of magnetic order but, instead, facilitates a large number of different ordering structures such as antiferromagnetic, stripe or spiral patterns depending on filling n , interaction strength U , and temperature T . According to RPA calculations for the ground state ($T = 0$) phase diagram in Ref. [73] these phases are separated by either sharp second-order phase transitions or regions of phase separation. Since some of the regions with a well-defined ordered ground state are rather narrow in the U vs n phase diagram we have carried out RPA calculations at finite temperature to identify the fillings where a stable ordered phase is expected to exist also at $T > 0$.

In a first step, we have investigated $n = 1.0$ for which the U vs T phase diagram is shown in the left panel of Fig. 12. The filled circles indicate the RPA transition temperature to an magnetically ordered state whereas the color corresponds to the ordering vector $\mathbf{q}_N$. While at low values of U no order emerges due to the strong geometrical frustration, we observe a finite transition temperature T for $U \gtrsim 0.6$. As the different colors of the transition points indicate, the ordering vector $\mathbf{q}_N$ changes for virtually any U which is incompatible with a well-defined ordered state. This is consistent with the ground state analysis from Ref. [73] where $n = 1.0$ marks a transition line between various ordered, incommensurate and phase separated states in the U vs n phase diagram.

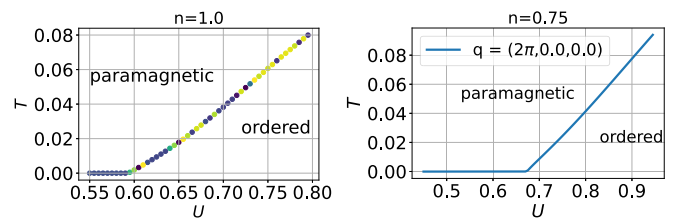


FIG. 12. RPA U vs T phase diagram of the fcc lattice at $n = 1.0$ (left panel) and $n = 0.75$ (right panel). In the left panel, different colors of the transition points indicate different ordering vectors.

We have, hence, carried out calculations also for $n = 0.75$ where the mean-field results of Ref. [73] predict a clear-cut ordered state at finite U with the ordering vector $\mathbf{q}_N = (0, 0, 2\pi)$ at $T = 0$. Our RPA data in the right panel of Fig. 12 confirm that such a stable magnetic phase survives

also at finite temperatures for interaction values $U \gtrsim 0.65$ which is in reasonable good agreement with the before mentioned ground state results. Consequently, we have carried out our DMFT and ID Γ A calculations for this filling in our manuscript.

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