How correlations change the magnetic structure factor of the kagome Hubbard model

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The kagome Hubbard model (KHM) is a paradigmatic example of a frustrated two-dimensional model. While its strongly correlated regime, described by a Heisenberg model, is of topical interest due to its enigmatic properties in cuprate high-temperature superconductors [1], most studied case, the Hubbard model on the triangular lattice, exhibits only short-range antiferromagnetic correlations, such as the double-exchange interaction. As we will see below, for a magnetically frustrated model with next-nearest-neighbor coupling, DMFT finds a first-order Mott transition from a metal to a paramagnetic insulator at low temperatures. Nonlocal correlations drastically change the physics: while short-range antiferromagnetic correlations significantly reduce the critical interaction U, long-range antiferromagnetic correlations shift the MIT to much smaller interactions, even to U = 0 for a square-lattice Hubbard model with perfect nesting [21,22]. Hence, long-range antiferromagnetic correlations open a gap. This conclusion is corroborated by quantum Monte Carlo simulations on large finite lattices [21,23–25].

The situation becomes qualitatively different in the presence of frustration. As sizable ground-state degeneracy is typical for a frustrated model, magnetic instabilities may spread over different momenta, suppressing the overall tendency toward magnetic ordering. Ramifications for the MIT are surmised, but model-specific information is scarce. The most studied case, the Hubbard model on the triangular lattice, shows a conventional MIT even if nonlocal correlations are still considerably lower values of U. For two-dimensional lattices without perfect nesting, these results suggest a MIT at still considerably lower values of U. For two-dimensional lattices without perfect nesting, these results suggest a MIT at still considerably lower values of U. For two-dimensional lattices without perfect nesting, these results suggest a MIT at still considerably lower values of U.
intersite hopping amplitude in the strongly correlated limit of the Hubbard model (\(U \gg t\)) of the tight-binding kagome model with a positive \(J\). The blue line marks the chemical potential \(\mu\) on-site Coulomb repulsion of the noninteracting system is half filled.

Much less is known about less correlated regimes of the half-filled kagome Hubbard model (KHM). Dynamical spin correlations were studied using cluster DMFT on a \(N = 3\) site clusters \([66–68]\) where the first-order MIT occurs at \(U_c = 8.4t\) \([66]\). As noticed in Ref. \([69]\), a major drawback of odd-numbered clusters is their incompatibility with valence bond states. Instead, variational cluster calculations on \(N = 6\) and \(N = 12\) clusters demonstrate that the formation of intersite singlets (valence bonds) underlies the MIT and propels it to a smaller \(U\) value. In the weak coupling limit, determinant quantum Monte Carlo (DQMC) calculations reveal a saturation of magnetic correlations at low temperatures and a Curie-like behavior for a strong interaction \(U = 8t\) \([70]\). A recent study suggests that the KHM harbors a topologically nontrivial state, a higher-order topological Mott insulator, characterized by corner modes whose spin excitation spectrum is gapless \([71]\).

For a long time, the KHM attracted little attention: although potential modifications of herbertsmithite hold promise for unconventional phases \([72]\), pristine herbertsmithite and related quantum magnets \([73–75]\) are correlated insulators deep in the Heisenberg limit. The situation changed drastically after the discovery of metallic kagome materials Mn\(_3\)Sn \([76–81]\), Fe\(_3\)Sn\(_2\) \([82–90]\), Co\(_3\)Sn\(_2\)S\(_2\) \([91–100]\), Gd\(_3\)Ru\(_4\)Al\(_{12}\) \([101,102]\), and FeSn \([103–106]\). The potential of kagome systems to harbor superconductivity was elucidated by DQMC simulations long ago \([70]\). Very recently, the discovery of superconductivity in the new family of V-based kagome materials AV\(_3\)Sb\(_5\) \([107]\) (KV\(_3\)Sb\(_5\) \([108]\), RbV\(_3\)Sb\(_5\) \([109]\), and CsV\(_3\)Sb\(_5\) \([110]\)) resulted in a flurry of activity on the experimental as well as the theory side. At present, the magnetic properties of these materials remain largely enigmatic and even the presence of local moments is discussed controversially \([111,112]\). Despite the diversity of structural motifs and physical behaviors, a common trait of these materials is metallic conductivity concomitant with partially filled \(3d\) electronic shells whose contributions dominate in the low-energy sector. Hence, the key to their electronic and magnetic properties should be sought in less correlated regimes of the KHM, which remain hitherto largely unexplored.

In this paper, we fill this gap by performing an extensive numerical investigation of the KHM using three different many-body techniques: DQMC \([113]\), DMFT \([12,13]\), and the dynamical vertex approximation (D\(\Gamma\)A) \([114,115]\). DQMC is a numerically exact technique for fermionic lattice models. With the caveat that finite lattices beget finite size effects, it provides a sound benchmark for quantum impurity methods. Since frustration of the KHM gives rise to a severe sign problem, we restrict our DQMC calculations to relatively high temperatures. We use these results as a benchmark for D\(\Gamma\)A, a diagrammatic extension of DMFT. In contrast to cluster extensions of DMFT \([116]\), this method accounts for nonlocal correlations on all length scales—from short-range to long-range—and unlike many QMC-based techniques, diagrammatic extensions of DMFT are immune to the sign problem \([115]\), allowing us to explore more correlated regimes of the KHM also at lower temperatures. In this paper, we apply the recently implemented self-consistent D\(\Gamma\)A scheme \([117]\), which eliminates the need to restore the sum rules by means of so-called \(\lambda\) corrections \([118,119]\).

Our main finding is the gradual correlation-induced change in the regime of magnetic correlations: While maxima at the \(K\) point of the extended Brillouin zone (BZ) are indicative of dominant \(\sqrt{3} \times \sqrt{3}\) correlations, the enhancement of interaction strength gives rise to the sign change of third-neighbor correlations. Interestingly, this crossover occurs in the metallic phase, while spin correlations in the moderately correlated...
regime are similar to those of the Heisenberg model. This finding gives us a key to distinguish between weakly and strongly correlated regimes in the growing family of kagome materials. Furthermore, we compute the dynamical structure factors $S(q, \omega)$ for different regimes of the KHM. Since these quantities are accessible in inelastic neutron scattering experiments, the relative strength of electronic correlations in real materials can be estimated by a direct comparison to our calculated $S(q, \omega)$.

Our paper is equally important for method development in the field of electronic correlations: it applies a diagrammatic beyond-DMFT method, DΓA, to a strongly frustrated two-dimensional model. Extensive comparisons with the numerically exact lattice-based method (DQMC) reveal an overall good agreement, indicating that a self-consistent DΓA calculation captures the leading effects of nonlocal fluctuations, even if tendencies toward magnetic ordering are strongly suppressed.

This paper is organized as follows. In Sec. II, we introduce the Hubbard model on a kagome lattice and briefly explain the methods we use to obtain our results. The main results are presented in Sec. III, where we first present the phase diagram and then discuss the magnetic structure factors. In Sec. IV, our results are compared to previous theoretical results from the literature and put in the context of present-day experimental research. We summarize our results in Sec. V. Additionally, we provide more detailed information about the influence of certain real-space correlations on the structure factor in the Appendix.

II. NUMERICAL METHODS

A. KHM Hamiltonian

We define the Hamiltonian of the Hubbard model on a kagome lattice as

$$H = \frac{1}{V_{BZ}} \int d{k} \sum_{j,l,\sigma} h_{jl}(k)c_{j\sigma}^\dagger(k)c_{l\sigma}(k) + \sum_{k} \sum_{\mathbf{R}} u_{\mathbf{R},j} n_{\mathbf{R},j\uparrow} n_{\mathbf{R},j\downarrow}, \tag{1}$$

where $V_{BZ}$ is the volume of the BZ [Fig. 1(b)], $\mathbf{k}$ is the 2D crystal momentum, and indices $j$ and $l$ refer to the sites within the unit cell and run from 1 to 3. The three sites comprising the unit cell [as shown in Fig. 1(a)] form an equilateral triangle whose side length is half of the lattice constant. The tight-binding Hamiltonian $h_{jl}(k)$ incorporates the lattice geometry and hopping amplitudes. In the second term, we have a sum over all unit cells, where site $j = 1$ is located at the Bravais lattice position $\mathbf{R}$. The interaction, parametrized by a scalar $U$, is of density-density type.

As hopping is allowed only between neighbor sites, the noninteracting part of the Hamiltonian reads

$$h_{jl}(k) = -t \begin{pmatrix} 0 & 1 + e^{ik_1} & 1 + e^{ik_2} \\ 1 + e^{-ik_1} & 0 & 1 + e^{-ik_1-k_2} \\ 1 + e^{-ik_2} & 1 + e^{ik_1-k_2} & 0 \end{pmatrix}, \tag{2}$$

where $k_1$ and $k_2$ are the projections of $k$ onto the reciprocal basis vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. We set the hopping amplitude to unity $t = 1$, which defines our unit of energy used throughout the paper. By further setting $\hbar = 1$ and $k_B = 1$, we also fix the units of frequency and temperature.

By applying a unitary transformation $U(k)$, the Hamiltonian matrix Eq. (2) can be diagonalized,

$$h(k) = U(k) \underline{\epsilon}(k) U^\dagger(k), \tag{3}$$

where $h$ and $U$ are $k$-dependent matrices of dimension three, $\underline{\epsilon}$ is a $3 \times 3$ identity matrix, and $\underline{\epsilon}$ is a $k$-dependent three-dimensional vector, defining the tight-binding bands. The latter are shown in Fig. 1(c).

Evaluation of eigenenergies of the full Hubbard Hamiltonian Eq. (1) is not possible: the tight-binding term and the interaction term do not commute. We are therefore restricted to a handful of numerical methods that allow us to calculate correlation functions within a certain approximation. In this paper, we use three many-body methods to compute properties of the Hubbard model on a kagome lattice: DMFT, DΓA, and DQMC. Since the kagome lattice is not a standard application of these methods, we briefly review how they work in this case in order to prevent confusion.

B. Dynamical mean-field theory

DMFT utilizes the equivalence of the Hubbard model in infinite dimensions to an Anderson impurity model. The latter is amenable to an exact numerical evaluation of correlation functions. The pertinent hybridization function of the (auxiliary) Anderson impurity model is determined self-consistently [13]. While DMFT self-energies are frequency dependent, they lack momentum dependence, i.e., they are local.

Although DMFT workflows are exhaustively described in literature, we nevertheless provide an outline of our calculation scheme for the sake of clarity. In each step of a DMFT calculation, the four following operations are performed:

1. Calculate the local Green’s function $G_{loc}(i\omega_n)$ for the Hubbard model:

$$G_{loc}(i\omega_n) = \frac{1}{V_{BZ}} \int d{k} [(i\omega_n + \mu - \Sigma(i\omega_n))\underline{1} - h(k)]^{-1}. \tag{4}$$

At this step, the chemical potential $\mu$ is adapted to keep the system half filled. Note that the local Green’s function $G_{loc}(i\omega_n)$ at fermionic Matsubara frequency $\omega_n$ is still a matrix with respect to the three $j$ sites at Bravais lattice site $\mathbf{R} = 0$, whereas the self-energy $\Sigma(i\omega_n)$ is scalar multiplied with the $3 \times 3$ unit matrix $\underline{1}$.

2. Calculate the noninteracting Green’s function $\mathcal{G}_{j}(i\omega_n)$ for the impurity model at site $j$ within the unit cell:

$$[\mathcal{G}_j(i\omega_n)]_{11}^{-1} = ([G_{loc}(i\omega_n)]_{jj})^{-1} + \Sigma(i\omega_n). \tag{5}$$

where $\mathcal{G}_j(i\omega_n)$ is the local Green’s function for the $j$ site within the unit cell.
This $G_r(i\omega_n)$ defines three (equivalent) impurity problems
for each site $j$ of the unit cell, consistent with the DMFT
approximation.

(3) Calculate the self-energy $\Sigma(i\omega_n)$ of the impurity mod-
elves defined in step 2 by an impurity solver. To this end, we use
the numerically exact continuous-time quantum Monte Carlo
algorithm in the hybridization expansion [121]. Since all three
impurities are equivalent, we need to do this calculation only
once, thus saving computational time.

(4) Insert the self-energy $\Sigma(i\omega_n)$ of step 3 into the expres-
sion for the Green’s function $G_{\text{loc}}(i\omega_n)$ in step 1 and iterate
until convergence.

Our calculations were carried out by the program package
W2DYNAMICS [122]. Although we are solving a three-band
model, the downfolding approximation reduces the numerical
cost of the DMFT calculation roughly to that of a one-band
calculation. By using symmetric improved estimators [123],
our DMFT calculations converge very precisely and the result-
ate and strongly correlated regimes the Hubbard
functions show a rapid decay on the length scale equal to half
the bandwidth, for instance, near-neighbor
correlation functions are usually converged to a few percent
on lattices of linear extent $L \sim 10$. In the present case, compu-
tations were done for clusters of $5 \times 5$ unit cells (i.e., 75 sites).
We note that finite-size effects can be efficiently suppressed by
using twist-averaged boundary conditions [127,128]. While
it is desirable particularly for low $U$ values, in the moder-
ately and strongly correlated regimes the Hubbard $U$ mitigates
finite-size effects. DQMC calculations also have Trotter errors
proportional to the square of the discretization interval of the
inverse temperature $\beta = 1/T$. In our paper, Trotter errors are
of the same order as, or smaller than, the statistical errors from
the Monte Carlo sampling. Finally, as noted earlier, DQMC
calculations are limited by the sign problem [129,130].
A rough rule of thumb is that DQMC can be done down to
temperatures $T \sim W/30$, where $W$ is the bandwidth, for
interaction strengths $U \sim W$.

Since correlation functions in DQMC are computed di-
rectly in the real space, the necessary postprocessing includes
a Fourier transformation to the momentum space. This is in
contrast to DMFT and DΓA, where we obtain our results
directly in the momentum space. Provided that the correlation
functions show a rapid decay on the length scale equal to half

(2) Combine $F_d$ and $F_m$ to a crossing symmetric vertex $F$
as explained in Ref. [125].

(3) Compute the momentum-dependent self-energy by the
equation of motion, which schematically reads

$$\Sigma(k) = \frac{1}{2} U n + \frac{1}{\beta^2} U G G F G.$$  \hspace{1cm} (6)

The first term is the static (Hartree) contribution, the second one
contains the diagrams of higher order.

(4) Construct a new lattice Green’s function $G$ by

$$G(k, i\omega_n) = [(i\omega_n + \mu)1 - h(k) - \Sigma(k, i\omega_n)]^{-1}.$$  \hspace{1cm} (7)

Similar to DMFT, the chemical potential $\mu$ can be (slightly)
adapted to keep the system half filled. This Green’s function is
now used as a propagator in step 1 and the steps are repeated
until convergence in $\Sigma$.

After convergence is reached, we obtain the self-energy
$\Sigma(k, i\omega_n)$, which is a full $3 \times 3$ matrix in the space of
the three lattice sites of our basis and also depends, in addition to
the fermionic Matsubara frequency, on the crystal momentum
$k$. A similar procedure for unit cells with multiple equivalent
one-orbital impurities was also proposed for the dual fermion
approach [126].

C. Dynamical vertex approximation

The DΓA [114,115] is a method based on Feynman dia-
grams. Compared to DMFT, where the self-energy is local,
DΓA goes one step further and imposes locality on the ir-
reducible two-particle vertex. The Bethe-Salpeter equation
combines these local building blocks by nonlocal propagator
lines and leads to a momentum dependence in the suscepti-
bility. A momentum-dependent self-energy is then obtained via
the Schwinger-Dyson equation of motion. In our calculations,
we use ladder DΓA, where nonlocal fluctuations are con-
sidered only in the density (charge) and the magnetic (spin)
channel. In the following, we sketch the DΓA procedure in a
compact tensor notation, suppressing the frequency and for the
lattice quantities momentum and three basis site indices: the
interested reader will find a more detailed description in
Ref. [125] and particularly in Ref. [117].

The main input of a DΓA calculation is, besides the tight-binding
Hamiltonian, the irreducible vertex $\Gamma_{\alpha}(\Gamma_m)$ in the
density (magnetic) channel. It is computed from the
generalized susceptibility $\chi$ of the DMFT impurity by the
Bethe-Salpeter equation

$$\Gamma_r = \beta^2 (\chi_r^{-1} - \chi_0^{-1}).$$  \hspace{1cm} (4)

where $r$ denotes the channel. Note that the inversion is done
only with respect to fermionic Matsubara frequencies, since
the impurity problem has no orbital degrees of freedom. Next,
we perform the following iterative procedure [117]:

(1) Calculate momentum-dependent reducible vertices $F_d$
and $F_m$ for the kagome lattice by the Bethe-Salpeter equation

$$F_r = \left[1 - \frac{1}{\beta}\Gamma_r G G \right]^{-1} \Gamma_r, \text{ with } r = d \text{ or } m.$$  \hspace{1cm} (5)

Here, the inversions pertain also to the site indices $j$ and $l$,
since $G$ is the Green’s function of the Hubbard model and thus
a $3 \times 3$ matrix.
of the finite lattice, we can approximately assume that in the infinite-lattice model all longer-range correlations are zero. This allows us to do an interpolation in the momentum space, such that we can use the same momentum grid in all three methods. Spatial correlations, especially in the one-particle Green’s function, become shorter ranged if the interaction strength $U$ is increased. At $U = 5$ our maximally feasible cluster size of 75 sites leads to mild finite-size effects, noticeable as a peak broadening in the spectral function around the $\Gamma$ point in the bottom left panel of Fig. 4. However, no finite size effects are visible for stronger interactions.

III. RESULTS

We divide our results in two parts. In Sec. III A, we focus on the phase diagram of the KHM in the metallic regime and discuss how the spectral function evolves as a function of the interaction strength and temperature. While it is a common way to describe the physics of a model, we surmise that from the experimental viewpoint such a discussion is largely disconnected from the physics of kagome materials: there is no recipe to extract the information on the interaction strength $U$ connected from the physics of kagome materials: there is no such estimation is impeded due to thermal broadening. In the same plot, we plot a rough estimate for $Z$ from DQMC, which is estimated as the fraction of the spectral weight located in the quasiparticle region. The latter is determined from the DMFT spectral function for the same $U$ value. For D$\Gamma$A, we calculate a momentum-dependent $Z$ which is presented in Fig. 5 below.

Another characteristic correlation-induced phenomenon is the formation of the Hubbard bands—two incoherent spectral features separated by $\sim U$. As these bands are strongly asymmetric, we estimate their position by

$$
\omega_{\text{upper/lower}} = Z_{\text{DMFT}} \times \omega_{\text{max/min}} \pm \frac{U}{2},
$$

where $\omega_{\text{max/min}}$ are the upper/lower band edge of the tight-binding Hamiltonian, i.e., $2 - \mu_{\text{th}}$ and $-4 - \mu_{\text{th}}$. This heuristic formula interpolates between the noninteracting regime and the strongly correlated insulating regime where the Hubbard bands are at $\pm \frac{U}{2}$. It accounts for the fact that the separation of the Hubbard bands is more than $\pm U$ at small $U$ and describes the position of the Hubbard bands in Fig. 2 very well.

Next, we discuss the momentum-resolved spectral functions in Fig. 4. In the case of weak interaction ($U = 3$, left column of Fig. 4), all three methods basically reproduce the non-interacting tight-binding bands; the sole correlation effect is the quasiparticle broadening of the peaks. In the case of a stronger interaction ($U = 6$, right column of Fig. 4), we
still consistently obtain a metallic solution in all the methods. In DMFT, the spectral function shows the Fermi liquid behavior, with a renormalized tight-binding band structure and distinct Hubbard bands. However, nonlocal correlations alter this picture: the DΓA calculations show a merging of the bottom edge of the quasiparticle band with the lower Hubbard band. Such waterfall-like structures have also been observed experimentally in angle-resolved photoemission spectroscopy of cuprate superconductors [132]. In DQMC, the lower Hubbard band is even further suppressed, and we almost recover the noninteracting band structure, albeit with a large broadening.

Looking at the upper Hubbard band in DMFT and DΓA (upper and middle panels in the right column of Fig. 4), we notice that in DΓA the upper Hubbard band moves to a lower energy, closer to the quasiparticle flat band. In DQMC, this is again slightly more extreme: the spectral weight of the upper Hubbard band moves further down in energy and is visible only as an extreme broadening of the quasiparticle flat band [133].

Altogether, this implies another interesting observation at $U = 6$ (right column of Fig. 4): In DMFT, the whole band structure is renormalized so the distance between the Dirac crossing and the flat band at the $K$ point is reduced to approximately half the noninteracting value (compare also Fig. 5). Surprisingly, the inclusion of nonlocal correlations in DΓA increases the width of the middle band with respect to DMFT. Thus the gap size at the $K$ point, between Dirac crossing and flat band, is increased and in DQMC it even reaches its tight-binding value.

We can extract more insights by comparing the DMFT and DΓA self-energies. In DMFT, the self-energy is diagonal with respect to the three basis-lattice sites $j$; all three diagonal elements are even identical and there is no off-site contribution within DMFT. In DΓA, the diagonal elements are almost identical to the DMFT self-energy and show only a weak dependence on the momentum. The main difference is the presence of sizable off-diagonal elements that are strongly momentum dependent.

Analysis of matrix-valued quantities computed on the Matsubara axis is not straightforward. Often in such cases one considers the eigenvalues of the quantity. However, complex eigenvalues of a matrix are returned by numerics libraries in an arbitrary order, which makes further analysis, such as analytical continuation, even more complicated. In the case of the KHM, however, we (numerically) find that the eigenvalues of the DΓA self-energy at a certain frequency $i\omega_n$ and momentum $\mathbf{k}$ can be obtained by projecting it onto the eigenvectors of the tight-binding dispersion matrix Eq. (2) at the same momentum $\mathbf{k}$. For DMFT, this is fulfilled trivially, as $\Sigma$ is $\mathbf{k}$ independent and proportional to the $3 \times 3$ unit matrix for the three sites of the unit cell. In DQMC, we do not have direct access to the self-energy but from the fact that the lattice Green’s function approximately fulfills the property, we can conclude that this holds for the self-energy as well.

This projection relation implies that the tight-binding bands are mapped onto interacting quasiparticle bands with associated Hubbard bands, but they are not mixed by nonlocal correlations because the interaction is local. The momentum dependence entails that the self-energy in the band basis is, albeit diagonal, no longer proportional to the unit matrix as in the DMFT. This leads to a momentum- and band-dependent, but still well-defined, quasiparticle renormalization factor $Z_\alpha(\mathbf{k})$, where $\alpha$ is the band index. We show this quantity for $U = 6$ and $T = 1/3$ in Fig. 5. Since smaller $Z$ implies stronger renormalization, it explains why the lowest-lying quasiparticle band merges with the lower Hubbard band at $\Gamma$, the center of the BZ.

Let us compare these results with the well-studied Hubbard model on a square lattice. There, antiferromagnetic fluctuations dominate the phase diagram at all temperatures, leading to an insulating antiferromagnetic state even at smallest values...
of the interaction $U$ [21] in the limit of zero temperature. Looking at the magnetic susceptibility of the kagome lattice, we have to keep in mind that it is defined as

$$\chi_{\text{m}}^\mu(\mathbf{q}, i\omega_n) = \sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}} \int_0^{\beta} d\tau e^{i\omega_n\tau} \langle S^\mu_{\mathbf{R}}(\tau) S^\mu_0(0) \rangle, \quad (10)$$

i.e., it is a $3 \times 3$ matrix for each momentum and frequency. For numerical and technical reasons, our DfA calculations are restricted to $(S^z/S^z)$ correlation functions, which yield the standard magnetic susceptibility. Note that in the absence of magnetic field, diagonal correlations are equal to one-third of full correlations: $\langle S^z/S^z \rangle = \frac{1}{3} \langle S^z \cdot S^z \rangle$. Without symmetry breaking, and as we will see below, there are no signs of any long range order, spin-off-diagonal correlation functions such as $\langle S^y/S^0 \rangle$ or $\langle S^z/S^z \rangle$ vanish [134].

For a quantitative analysis, we resort to the eigenvalues of $\chi_{\text{m}}^\mu$. Similar to the case of the self-energy before, we again (numerically) find that the eigenvalues of the susceptibility matrix at frequency $i\omega_n$ and momentum $\mathbf{k}$ can be obtained by projection onto eigenstates of the tight-binding dispersion matrix Eq. (2). Thus the eigenvalues can be associated with the respective tight-binding bands. In Fig. 6, we show the (projected) eigenvalues of the zeroth Matsubara frequency on the q plane for $U = 3$ at high and low temperatures.

Notably, the dominant mode of the susceptibility is the one that corresponds to flat-band eigenstates. At high temperature it is flat, but develops an inconspicuous structure at lower temperatures. This is in agreement with cluster DMFT studies [66,68] for the presented values of $U = 3$ and $U = 6$. Importantly, Fig. 7 reveals that the maximal value of the susceptibility does not increase significantly as the temperature is lowered. Thus, our results seemingly contradict the early DQMC study in Ref. [70] that finds a Curie-like temperature dependence for $U = 8$. However, in the temperature range down to $T = 0.25$ which was studied there, our results also show an increasing susceptibility. Therefore, in sharp contrast to the square [22] and the triangular lattice [135], the KHM does not show any visible tendency toward magnetic ordering. Instead, the flat structure of the magnetic susceptibility indicates short-ranged spin fluctuations.

### B. Structure factors

Structure factors are, on the one hand, inherently connected with magnetic susceptibilities and, on the other hand, can be addressed experimentally, e.g., by neutron spectroscopy. Following the work on the Heisenberg kagome model [136,137], we calculate the equal-time structure factor $S_0(\mathbf{q})$ given by

$$S_0(\mathbf{q}) = \sum_{j,l} e^{i\mathbf{q}(\mathbf{r}_j-\mathbf{r}_l)} \sum_{\omega_n} \chi_{jl}(\mathbf{q}, i\omega_n) \quad (11)$$

and the dynamical structure factor $S(\mathbf{q}, \omega)$ given by

$$S(\mathbf{q}, \omega) = \frac{-\text{Im} \sum_{j,l} e^{i\mathbf{q}(\mathbf{r}_j-\mathbf{r}_l)} \chi_{jl}(\mathbf{q}, \omega + i0^+)/\pi}{1 - e^{-\beta\omega}}. \quad (12)$$

In Eqs. (11) and (12), $\mathbf{r}_j$ denotes the position of the jth atom in the unit cell. Since the shortest distance between two sites ($\frac{1}{2}$) is twice smaller than the unit cell constant Eq. (1), the structure factor is periodic in the extended BZ [Fig. 1(b)]. The analytic continuation of Matsubara frequencies or imaginary time to real frequencies is performed using ANA_CONT [138,139] employing the maximum entropy method [140]. As a technical remark, we note that in DfA we can analytically continue the projected eigenvalues of the susceptibility matrix individually and then go back to the sublattice space, where the summation in Eq. (12) is carried out. In the following, we present our results for the extended BZ of Fig. 1(b). Unfolding the three eigenvectors of the first BZ (e.g., for the magnetic susceptibility in Fig. 6) yields a single eigenvector for the larger (extended) BZ. Figure 8 shows a smooth distribution of the equal-time structure factor over the extended BZ and a weak temperature dependence. In all plots, $S_0(\mathbf{q})$ grows as...
we move from the center toward the boundary of the extended BZ and forms round maxima at its corners [the K points in Fig. 1(b)]. To get a deeper insight into magnetic correlations, we return to real space and plot the equal-time susceptibility $\chi$ as a function of real-space vector $\mathbf{R}$ connecting two sites. As expected for a strongly frustrated model, the resulting pattern in Fig. 9 is dominated by two contributions: the on-site contribution, which is trivially positive and yields a momentum-independent shift, and sizable negative, i.e., antiferromagnetic, correlations between the nearest neighbors ($\mathbf{R} = \mathbf{R}_1$). As we show in the Appendix, the latter are largely responsible for the maxima at the K points.

More intriguing is the pattern formed by weak longer-range correlations. In particular, by doubling the four $\mathbf{R}_1$ vectors (Table I) that point to four (out of six) third neighbors on the kagome lattice. A key observation is that the second-neighbor correlations ($\mathbf{R}_2$) and the remaining two third-neighbor correlations ($\mathbf{R}_{3a}$) are ferromagnetic (blue circles in Fig. 9). In momentum space, shown in Fig. 8, this has the following effect: strong negative correlations at $\mathbf{R}_1$ create the peaks at the K points and positive correlations at $\mathbf{R}_2$ further increase them. The negative correlations at $\mathbf{R}_{3a}$ overcompensate the positive ones at $\mathbf{R}_{3b}$ and thus reduce the structure factor at the M points. Altogether this leads to well-separated peaks at the K points.

So far, we discussed the structure factor in the weakly correlated regime ($U = 3$). If we now increase the interaction $U$, we observe an apparent change, both in momentum (Fig. 10) and real (Fig. 11) space. While $S_0(\mathbf{q})$ is still peaked at the K points, the intensity grows over the entire boundary of the extended BZ. Again the behavior is understood better by looking at the lattice. Antiferromagnetic nearest-neighbor correlations still generate the dominating peaks at the K points, supported by $\mathbf{R}_2$ correlations. However, in the shell of third neighbors, now the positive correlations prevail and increase the structure factor at the M points, i.e., between the K points. This means that the peaks become slightly less separated. More quantitatively, the ratio between the structure factor at the M point and K point at $U = 3$ is $0.87$ (0.85) in DQMC (DF) and it increases to $0.90$ (0.87) at $U = 6$.

Interestingly, our patterns are in excellent agreement with the equal-time structure factor computed using numerical linked cluster expansion for the Heisenberg kagome model [137]. We will discuss the ramifications in Sec. IV.

Since our calculations provide direct access to dynamical quantities, it is instructive to inspect the energy dependence of the structure factors. In Fig. 12, we plot the dynamical structure factor $S(\mathbf{q}, \omega)$ on a path through the extended BZ (Fig. 1) at weak interaction $U = 3$ for two different vectors.
temperatures. In line with the equal-time structure factor, the dominant weight is located around the $K$ point. Additionally, there is a splitting into a low- and high-energy mode at the $M$ point [cf. Fig. 1(b)], although at high temperature it is concealed by thermal broadening in DΓA.

Finally, we present the evolution of the dynamical structure factor as a function of correlation strength in Fig. 13. The main effect is squeezing the frequency spread of the intensity to lower energies accompanied by a gradual dissipation of spectral features. Note that it was not possible to converge a self-consistent DΓA calculation for the $U = 10$ case, and in DMFT the spectral weight is pushed to zero energy.

IV. DISCUSSION

Diagrammatic extensions alleviate the main drawback of DMFT—its restriction to local correlations. An alternative route to include nonlocal correlations are cluster extensions of DMFT. In the conceptually simple cellular DMFT (CDMFT) approach, such clusters are constructed in real space and typically comprise a small number of sites. Correlations in CDMFT are still purely local but the locality now spans the entire cluster. As a result, nonlocal correlations at the length scale of the cluster are included, while longer-range fluctuations are still absent. In addition to this sharp cutoff between the short-range (included) and long-range (omitted) correlations, CDMFT introduces a spurious disparity between the sites falling within the cluster and all other sites. We can illustrate this by considering the kagome lattice, where each site has four equivalent nearest neighbors. In the simplest possible cluster, a triangle, this equivalence is violated: only two of the four neighboring sites belong to the cluster. Keeping these intrinsic limitations of CDMFT in mind, we compare the results of three different CDMFT studies \cite{66,141,142} with our DΓA and DQMC results.

In three-site CDMFT employing a Hirsch-Fye impurity solver, Ohashi et al. reported a first-order transition at the critical $U_c = 8.22$ \cite{66}. While we were not aiming at a precise estimate for the critical interaction strength, the three-site CDMFT values is somewhat lower than our DMFT value and higher than our DQMC estimate with 75 sites (and no DMFT bath).

In the strongly correlated regime ($U = 6, 6$), the largest eigenvalue of the magnetic susceptibility plotted as a function of $q_x$ is nearly flat in CDMFT, with shallow minima along the six $\Gamma$-$M$ lines. Precisely, this behavior is observed in the DΓA susceptibility (Fig. 6). Interestingly, Ohashi et al. report a drastic change of magnetic correlations in the insulating phase: they argue that a starlike structure in the structure factor...
indicates the onset of 1D antiferromagnetic correlations [66]. We believe that this is an artifact of CDMFT. This is corroborated by the fact that the spin correlations that we obtain in DΓA and DQMC for the moderately correlated regime of the Hubbard model are similar to those of the Heisenberg model [137].

The more recent CDMFT study by Udagawa and Motome [141] employs a continuous-time auxiliary-field QMC impurity solver and uses, in addition to triangles, also more extended nine-site clusters. While the density matrix defined from microscopic states of a cluster is not accessible in the diagrammatic extensions, our temperature-dependent susceptibility (Fig. 7) agrees with the CDMFT results plotted in Fig. 4(d) of Ref. [141], except for the lowest temperatures, where we do not find the downturn of χ(T) characteristic for antiferromagnetic correlations or the formation of localized dimers. While not much is known for the KH, we note that in the kagome Heisenberg model, dimer tunneling processes around the loops comprising eight sites play a pivotal role [143]. The absence of such loops in the nine-site clusters used in Ref. [141] may give rise to the formation of static antiferromagnetic dimers, and hence a suppressed susceptibility.

Finally, Kita et al. focused on the behavior of the KH in a magnetic field [142]. Nevertheless, it is instructive to discuss their CDMFT spectral function in zero field, computed for U = 4 and U = 8 (Fig. 1 in Ref. [142]). The former agrees well with our DΓA results for U = 3, except for the substantial broadening in the CDMFT data at low frequencies, which might be an artifact of analytic continuation. The U = 8 case is more interesting. Here, in contrast to single-site DMFT and in agreement with DΓA, no distinct lower Hubbard band is formed; instead, a dispersive feature stemming from the lowest-lying branch of the kagome band structure shows up at low frequencies. Close to the Fermi level, two narrow, nearly dispersionless bands form in CDMFT [142]. We do not observe such structures in our U = 6 calculations, neither in DΓA, nor in DQMC: the intensity maxima lie above the Fermi level. At higher frequencies corresponding to the upper Hubbard band, CDMFT shows a broad spectral maximum in the vicinity of the Γ point which rapidly decreases for finite momenta. A similar, albeit less pronounced broadening of the spectral weight is visible in DΓA results (Fig. 4): the intensity at the Γ point is maximal.

Structure factors are a direct source of information on the dominant magnetic correlations and instabilities. A prominent example is the antiferromagnetic instability of the square-lattice Hubbard model, signaled by the diverging structure factor at q = (π, π), the propagation vector of the Néel state. In contrast, the structure factors of the KH in the metallic regime lack any apparent instabilities and instead show an intricate evolution on the frequency/momentum grid. Thus, to get insights into the magnetic correlations, we compare the behavior of S(q) and S(ω) with the literature data for the Heisenberg model.

The kagome Heisenberg model features several low-lying states with marginally different energies. While the debate on the ground state is still not settled, structure factors recently came into the forefront as a possible fingerprint to distinguish these states experimentally. A popular strategy is to pick a certain candidate state and calculate its structure factor using various mean-field techniques [31,50,136,144–147]. However, in the context of our paper, a more appropriate starting point is the direct simulation of the Heisenberg model on a finite lattice, followed by the evaluation of structure factors from the spin correlations. Regardless of the method used, the resulting S(q) of the Heisenberg model smoothly evolves from the minimum at Γ to the maximum at the boundary of the extended BZ. Further details depend on the computational method: While exact diagonalization on 36-site finite lattices yields feeble yet discernible peaks at M [148,149], these features are practically wiped out in density-
matrix renormalization group simulations [39,150] that are less prone to finite-size effects. The featureless structure factor indicates that tendencies to ordering are strongly suppressed, even on a short range. Since they arise from competing correlations, this balance can be destroyed by small deviations from the Heisenberg model, such as anisotropies and/or longer-range exchanges. A common ramification is the appearance of maxima at $K$ or $M$ points of the extended BZ, indicative of so-called $[151] \sqrt{3} \times \sqrt{3}$ or $q = 0$ antiferromagnetic correlations, respectively.

We are now in a position to compare the equal-time structure factors of the KHM in Figs. 8 and 10 with that of the Heisenberg model. First, the smooth $q$-evolution and the minimum at $\Gamma$ are common for both models. For all studied $U$ and $T^*$ values, the maximal intensity is at $K$, indicating the predominance of $\sqrt{3} \times \sqrt{3}$ correlations. This is seemingly at odds with the Heisenberg model, where weak maxima, if any, are found at $M$ $[148,149]$. However, a key difference lies in the methods: we do calculations at finite temperature. Looking at the finite-temperature structure factors for the Heisenberg model $[137]$, we see a strikingly similar picture: a smooth evolution with maxima at $K$. This brings us to one of the main conclusions: at moderate temperatures, the magnetic correlations of the KHM are similar to those of the Heisenberg model. Recently, a similar trend has been discovered in a dual-fermion study of the Hubbard model on the triangular lattice $[135]$. While the insensitivity of magnetic correlations to the MIT is likely related to geometrical frustration, we remind the reader that in contrast to KHM the triangular-lattice model has a ordered, three-sublattice ground state in the Heisenberg limit.

While our equal-time structure factors are quantitatively similar in the weakly and strongly correlated regime (cf. Figs. 8 and 10), real-space plots of respective susceptibilities reveal a subtle change in third-neighbor correlations (cf. Figs. 9 and 11). At weak coupling ($U = 3$), Fig. 11 shows along the direction of the two Bravais lattice vectors a negative($R_1$)-negative($R_{\pi}$)-positive spin correlation function, hinting at tendencies toward a $120^\circ$ spin-orientation. At strong coupling ($U = 6$ and $U = 10$), the third-nearest neighbor ($R_{3\pi}$) changes sign. In the half-filled one-band Hubbard model with a strong negative (antiferromagnetic) preference between nearest neighbors, this is arguably the most dramatic change one might expect, devoid an actual ordering that is prevented by the frustrated lattice. Note that the third-nearest neighbors and second-nearest neighbors are both at a distance of two hopping elements, they only differ by their distance in real space because of the geometry.

We attribute this difference to the correlation-induced onset of $q = 0$ magnetic correlations that compete with dominating $\sqrt{3} \times \sqrt{3}$ correlations. At the same time, susceptibilities in the moderately correlated regime (Fig. 11) are qualitatively similar to those in the Heisenberg model $[137]$, where the sign of the correlation function is determined by the Manhattan distance $[152]$. Therefore, we conclude that $q = 0$ correlations already develop in the moderately correlated regime, i.e., in the metallic phase. This nontrivial result provides a key to distinguish between the weakly and moderately correlated regimes in real materials: The former features predominantly $\sqrt{3} \times \sqrt{3}$ correlations, while in the latter additional $q = 0$ correlations become manifest.

Next, we discuss the features of the dynamical structure factor $S(q, \omega)$. While details of the plots are prone to uncertainties of the analytic continuation, we comment on one salient feature: the difference between the frequency dependencies at $K$ and $M$. The highest spectral density is associated with $K$ (consistent with the maxima in the equal-time structure factor), but is shifted to higher frequencies as compared to $M$. Interestingly, the same structure is found in the structure factor of a $\mathbb{Z}_2$ spin liquid with a moderate spinon-vison interaction $[136]$. Our paper should motivate further studies to clarify whether metallic kagome magnets can serve as a playground for topological vison excitations, which have been suggested in Ref. [136].

Finally, we put our results in the context of ongoing experimental activities on metallic kagome magnets. While we computed the quantities that can be measured by inelastic neutron scattering, several aspects impede a direct comparison. First, all so-far discovered metallic kagome materials are multiorbital systems. A simplified effective one-orbital description is generally possible, but the mapping scheme depends on the specifics of a particular material and has to be adjusted accordingly. Second, a kagomelike arrangement of magnetic atoms in the crystal structure does not guarantee the applicability of the KHM: coupling beyond nearest neighbors as well as interplane couplings can play a significant role. This is the case for Mn$_2$Sn, where neutron-scattering experiments reveal the relevance of multiple magnetic exchanges $[104]$. Bilayer kagome systems Fe$_2$Sb$_2$ $[90]$ and Co$_2$Sb$_2$ $[100]$ that entail a sizable interlayer coupling fall in the same category. Also, the band filling, whose estimation in a real material is per se challenging, can deviate from the case in point: KHM at strict half filling. All in all, we believe that presently the most promising case is FeSn, whose band structure (Fig. 4 in Ref. [104]) bears apparent similarities to the half-filled tight-binding kagome model. We are looking forward to future inelastic neutron-scattering experiments (announced in Ref. [106]) that can be compared with our structure factors and dynamical susceptibilities. Potentially even more promising are V-based $AV_3Sb_5$ ($A = K, Rb, Cs$) materials $[107–112,153,154]$, yet more experimental information on their magnetism is urgently needed.

V. CONCLUSION

We studied the phase diagram and the magnetic structure factor of the KHM, focusing on the weakly and moderately correlated regime relevant for the growing family of real materials. To this end, we employed three complementary methods: DMFT, DΓA, and DQMC. We observe neither tendencies toward magnetic ordering of any kind nor fingerprints of singlet formation. To provide solid reference data for inelastic neutron-scattering experiments on candidate materials, we calculate dynamical as well as equal-time structure factors and susceptibilities for a wide range of the interaction parameters $U$ and at different temperatures. By comparing our results with the literature data for the Heisenberg model, we conclude that the Mott transition is not accompanied by a sensible alteration of magnetic correlations: the major change
already happens in the metallic phase, where the magnetic coupling to third-nearest neighbors changes sign. We argue that this change gives a key to estimate $U$, and hence the proximity to a MIT, in real materials.

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FIG. 14. How certain real-space correlations influence the magnetic susceptibility and structure factor. In the first three columns, we show the projection of the magnetic susceptibility on the lower-band, middle-band, and flat-band eigenstates of the tight-binding Hamiltonian, respectively. The right-most column shows the corresponding structure factor $S(q)$ on the extended BZ. The rows correspond to various correlations in real space: Thus, in the first row we show momentum-space correlations arising from on-site correlations. The second row corresponds to nearest-neighbor correlations ($R_1$). The third, fourth, and fifth rows correspond to $R_2$, $R_3$ and $R_4$ correlations.
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**APPENDIX: FINGERPRINT OF REAL-SPACE CORRELATIONS**

For a better understanding of how spin-spin correlations between certain points in the lattice affect the susceptibility or structure factor in momentum space, it is helpful to study the connection analytically. The basis for this is Eq. (10), where we set \( (s^z_1(R, \tau) s^z_2(0, 0)) = 1 \) for a certain vector \( R \) and all vectors that are related by symmetry transformations. Figure 14 shows, row by row, how correlations to a certain neighbor \( R \) and its symmetrically related counterparts reflect in \( k \) space. The first three columns are the projections to tight-binding eigenstates and the fourth column is the structure factor.

Unsurprisingly, on-site correlations yield just a constant contribution. \( R_1 \) and \( R_2 \) correlations lead to peaks at the \( K \) point in the extended BZ, whereas \( R_3 \) correlations enhance the \( M \) point (last two rows in Fig. 14).

It is important to note that, for this analysis, we always consider positive correlations (of unit magnitude) between neighboring sites at the indicated distance, negative ones just change the sign. For the nearest-neighbor correlations \( (R_1) \) this means, e.g., that we get negative peaks at the \( K \) points, whereas the actual correlations at \( R_1 \) are negative yielding positive peaks around the \( K \) points. Furthermore, let us note that the number of neighbors at \( R_{1a} \) is twice as large as the number of neighbors at \( R_{1b} \). Therefore, their influence on the structure factor is also twice as large.

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