

Magnetic correlations in a periodic Anderson model with nonuniform conduction electron coordination

N. Hartman,¹ W.-T. Chiu,² and R. T. Scalettar²¹*Department of Physics, Southern Methodist University, Dallas, Texas 75275-0175*²*Department of Physics, One Shields Ave., University of California, Davis, California 95616, USA*

(Received 9 February 2016; published 21 June 2016)

The periodic Anderson model is widely studied to understand strong correlation physics and especially the competition of antiferromagnetism and singlet formation. In this paper we extend quantum Monte Carlo work on lattices with uniform numbers of neighbors to geometries in which the conduction electron sites can have variable coordination z . This situation is relevant both to recently discovered magnetic quasicrystals and also to magnetism in doped heavy fermion systems. Our key results are the presence of antiferromagnetic order at weak interorbital hybridization V_{fd} , and a delay in singlet formation to larger values of V_{fd} on sites with larger z . The staggered magnetization tends to be larger on sites with higher z , providing insight into the behavior to be expected in crown, dice, and CaVO lattices.

DOI: [10.1103/PhysRevB.93.235143](https://doi.org/10.1103/PhysRevB.93.235143)

I. INTRODUCTION

The single band Hubbard Hamiltonian [1–4] captures several of the most fundamental consequences of electron-electron interactions in solids, namely, magnetic order and the Mott metal-insulator transition. Multiband Hamiltonians like the periodic Anderson model (PAM) [5,6] examine what happens when two species of electrons, one delocalized “conduction” band (often d), and another localized band (often f), are present. Here a central effect is the competition between singlet formation [7], when the conduction and localized electrons are strongly hybridized, and ordering of the local moments mediated indirectly through the Ruderman-Kittel-Kasuya-Yosida interaction [8–11]. In heavy fermion materials [12,13], this competition is believed to explain different low-temperature phases, e.g., nonmagnetic CeAl₃ where the f moments are screened by the conduction electrons, and CeAl₂ which becomes antiferromagnetic (AF) at low temperatures.

Quantum Monte Carlo (QMC) studies of the PAM have explored some of this physics, in one [14,15], two [16], and three dimensions [17]. The focus has been on bipartite lattices which, at half-filling, host AF order without frustration and are also free of the fermion sign problem [18,19]. QMC in infinite dimensions [20] complements work in finite d by allowing simulations at very low temperature, at or even well below the Kondo scale, at the expense of some of the knowledge of correlations in space.

There is interest in understanding the magnetic correlations in more general geometries. One such modification allows for intersite, rather than on-site, hybridization between conduction and local orbitals and hence metallic behavior in the absence of interactions [21]. Another motivation is provided by chemical substitution in heavy fermion materials, either by the replacement of some of the local moment atoms by nonmagnetic ones, as in (Ce,La)CoIn₅ [22], or by changes to the conduction orbitals, as in the alloying of Cd onto In sites in CeCo(In,Cd)₅ [23]. In the latter situation, V_{fd} is reduced locally, and AF droplets can form around the impurity sites.

A second motivation is the recent observation of a quantum critical state in magnetic quasicrystals [24,25]. In these Au-Al-Yb alloys (Au₅₁Al₃₄Yb₁₅), measurements of the magnetic

susceptibility χ and specific heat C diverge as $T \rightarrow 0$. This non-Fermi-liquid (NFL) behavior is associated with strongly correlated $4f$ Yb electrons. These two sets of materials share a common feature which is that the coordination number of the different atoms is no longer spatially uniform. The effects of these unique local environments can be probed with nuclear magnetic resonance [26].

The NFL behavior of Au-Al-Yb alloys has recently been studied by solving the $U = \infty$ Anderson impurity model for a single local moment coupled to conduction electrons in a quasicrystal approximant geometry [27]. The crucial result is that singular responses in χ and C occur as a consequence of a broad (power-law) distribution of Kondo temperatures which delays screening of a large fraction of the magnetic moments until very low temperatures.

In this paper we study the PAM in two different geometries: the Lieb lattice and a two-dimensional (2D) “Ammann-Beenker” tiling [28,29]. Quasicrystalline approximants [30] for Au₅₁Al₃₄Yb₁₅ are in three dimensions; the quasiperiodic Ammann-Beenker tiling is a more tractable 2D alternative for QMC, which is limited in the number of sites which can be simulated.

Our goal here is to explore the nature of magnetic correlations as a function of f - d hybridization, and specifically, to understand the competition of antiferromagnetic order and singlet formation in geometries where the coordination number of different sites in the lattice is nonuniform. Our work extends that of [27] by examining a dense array of local orbitals and also by including the effect of finite U_f . We begin with the Lieb lattice, because it contains two separate coordination numbers, $z = 2, 4$, while still retaining very simple lattice periodicity. We then turn to the more complicated quasicrystal approximant structure. We do not at present address the anomalous NFL behavior of the magnetic susceptibility, since those phenomena appear to be associated only with the quasicrystal itself, and not its approximant [23].

The magnetic properties of quantum antiferromagnets in geometries which have a variable coordination number (quasicrystal, crown, and dice lattices) have also been studied in the context of the spin-1/2 Heisenberg Hamiltonian [31–34].

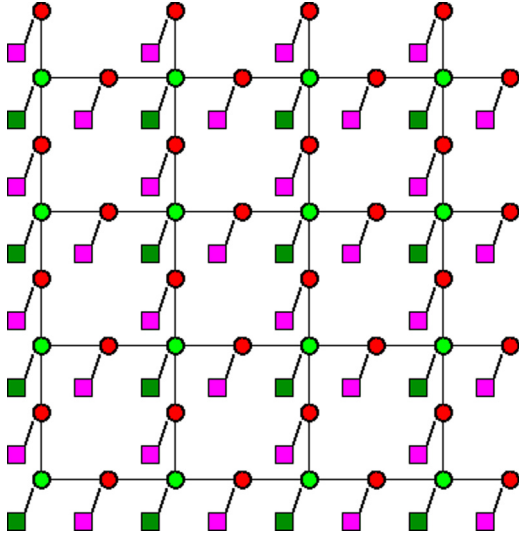


FIG. 1. The Lieb lattice geometry under consideration in this paper. (Cluster shown has 4×4 unit cells with 48 sites). Each site contains both a conduction (d) orbital (circles) and a localized (f) orbital (squares), so that there is a total of 96 sites/orbitals. Horizontal and vertical lines correspond to the d - d hopping t . We use periodic boundary conditions (PBCs). There are two possible conduction orbital coordinations, $z = 2, 4$. The local f orbitals are connected to the d orbital on the same site by hybridization V_{fd} (diagonal lines).

The general trend is to a reduction in order (e.g., the staggered magnetization) on sites with larger z . On the other hand, in the case of *regular* geometries with uniform z , the ordered moment *increases* from the honeycomb and CaVO ($z = 3$) to square ($z = 4$) lattices [35]. We observe the latter trend here: spin-spin correlations grow with z . We will comment on this further in our conclusions.

Similar issues of magnetic order in quasicrystal lattices have also been explored in classical models. Ising spins coupled by Ruderman-Kittel-Kasuya-Yosida interactions [36] exhibit the somewhat surprising result of a low-temperature phase with long-range order, as opposed to glassy behavior. As in the quantum cases mentioned above, and studied in our work below, the magnetism is strongly dependent on the local environment. Meanwhile, the magnetic order of classical Heisenberg spins on a quasicrystal lattice is explored in [37].

II. MODEL AND METHODS

The PAM is a tight-binding Hamiltonian for which each spatial site contains both an extended and a localized orbital,

$$\mathcal{H} = -t \sum_{(ij), \sigma} (d_{i\sigma}^\dagger d_{j\sigma} + d_{j\sigma}^\dagger d_{i\sigma}) - V_{fd} \sum_{i\sigma} (d_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger d_{i\sigma}) + U_f \sum_i \left(n_{i\uparrow}^f - \frac{1}{2} \right) \left(n_{i\downarrow}^f - \frac{1}{2} \right). \quad (1)$$

Here t is the hybridization between conduction orbitals with creation (destruction) operators $d_{i\sigma}^\dagger$ ($d_{i\sigma}$) on nearest-neighbor sites (ij). In this paper we consider the two conduction electron geometries shown in Figs. 1 and 2 corresponding to ‘‘Lieb’’ and

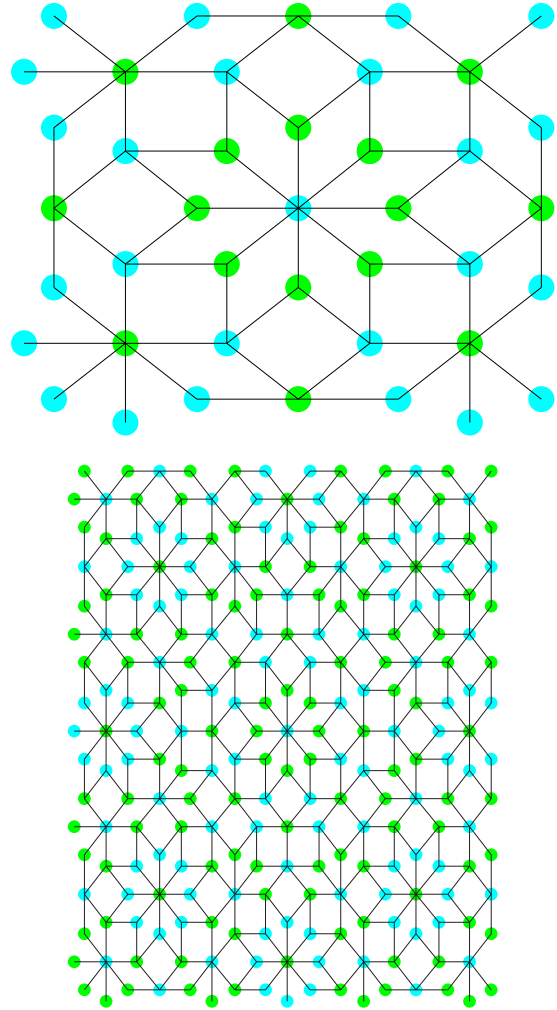


FIG. 2. Top (bottom): Approximants to the $\text{Au}_{51}\text{Al}_{34}\text{Yb}_{15}$ crystalline lattice for $N = 41(239)$ sites. In each case, sites shown contain both a conduction (d) orbital and a localized (f) orbital. Because of the more complex (irregular) structure, we show only the conduction sites (circles) explicitly. There is a partner localized site (not shown) for each, the analogs of the squares in Fig. 1. Lines correspond to the d - d hopping t . The local f orbitals are connected to the d orbital on the same site by hybridization V_{fd} . For this geometry we use open boundary conditions (OBCs) to avoid frustration. The conduction electron sites range in coordination from $z = 1$ to $z = 8$. The use of two colors for the sites emphasizes that, despite its complexity, the geometry is still bipartite.

‘‘quasicrystal’’ lattices, respectively. Each site of these lattices also contains a localized orbital, and creation (destruction) operators $f_{i\sigma}^\dagger$ ($f_{i\sigma}$). U_f is the on-site interaction between spin-up and spin-down electrons on the localized orbital, and V_{fd} is the conduction-localized orbital hybridization. Both geometries of Figs. 1 and 2 are bipartite. In \mathcal{H} we have written the interaction term, in ‘‘particle-hole’’ symmetric form, and set the site energy difference between f and d orbitals to zero, so that the lattice is half-filled for all temperatures T and Hamiltonian parameters t, U_f, V_{fd} . Half-filling optimizes the tendency for AF correlations, and also allows determinant Quantum Monte Carlo (DQMC) simulations at low temperature since the sign problem [18] is absent.

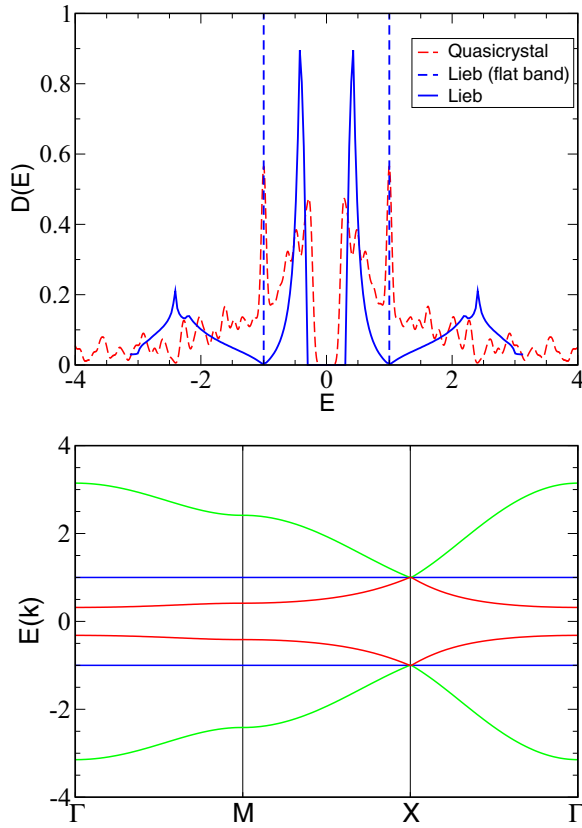


FIG. 3. DOS (top) and band structure (bottom) of the PAM on a Lieb lattice. Here $t = 1$ and $V_{fd} = 1$. The two completely flat bands at $E = \pm 1$ give rise to δ function spikes in $D(E)$ which are indicated by dashed vertical lines). $D(E = 0)$ vanishes: the system is a band insulator at half-filling. The DOS for the $N = 239$ quasicrystal approximant is also shown in the top panel. As is the case for the Lieb lattice PAM, the quasicrystal PAM also has a hybridization gap at $E = 0$. The single band case is metallic [27,34].

Figure 3 shows the density of states and band structure of the PAM on a Lieb lattice for $t = 1$ and $V_{fd} = 1$. There are six bands corresponding to the six sites (three conduction and three localized) per unit cell. The lattice is bipartite with four of the six sites on one sublattice and two on the other. Hence, in accordance with Lieb's theorem [38] there are two flat bands (at $E = \pm 1$). As in the case of the PAM on a square lattice with on-site hybridization, the half-filled lattice is a band insulator in the noninteracting limit. However, by comparing calculations for on-site and intersite V_{fd} , the latter being metallic at half-filling, it has been shown that many properties of the PAM when $U_f/t \gtrsim 4$ are insensitive to the presence of a $U_f/t = 0$ band gap [21].

The magnetic properties of the PAM are characterized by intra- and interorbital spin-spin correlations,

$$\begin{aligned} c_{ff}^{zz'}(r) &= \langle f_{i+r\downarrow}^\dagger f_{i+r\uparrow} f_{i\uparrow}^\dagger f_{i\downarrow} \rangle, \\ c_{dd}^{zz'}(r) &= \langle d_{i+r\downarrow}^\dagger d_{i+r\uparrow} d_{i\uparrow}^\dagger d_{i\downarrow} \rangle, \\ c_{fd}^{zz'}(r) &= \langle f_{i+r\downarrow}^\dagger f_{i+r\uparrow} d_{i\uparrow}^\dagger d_{i\downarrow} \rangle. \end{aligned} \quad (2)$$

Here the superscripts z, z' refer to the coordination number of the conduction orbital on site i and $i + r$, respectively.

This separation allows us to isolate the effects of the number of neighbors on the spin correlations [39]. We focus here on $c_{ff}^{zz'}(r)$ which measures intersite magnetic correlations between the local electrons, and $c_{ff}^{zz}(r = 0)$, the singlet correlator between local and conduction electrons on the same site. The spin-spin correlations are translationally invariant for uniform geometries and periodic boundary conditions, but depend more generally on both i and r in irregular lattices.

We also measure the structure factor,

$$\begin{aligned} S_{ff}^z &= \sum_r \sum_{z'} c_{ff}^{zz'}(r) (-1)^r, \\ S_{ff}^{\text{tot}} &= \sum_r \sum_{z, z'} g^{zz'} c_{ff}^{zz'}(r) (-1)^r, \end{aligned} \quad (3)$$

which sums the spin-spin correlations to all distances r from sites i with a given z . The staggered phase factor $(-1)^r$ takes the value ± 1 on the two sublattices of the bipartite geometry and hence measures AF order. The z -resolved contributions to the total structure factor S_{ff}^{tot} are weighted by the fractions of sites in the lattice with a given coordination $g^{zz'}$. In the singlet phase, the spin correlations decay exponentially with separation r and S_{ff}^{tot} gets contributions only from a small number $r < \xi$ of local correlations. It becomes temperature independent below a relatively high T set by the singlet energy scale. In an ordered phase, on the other hand, S_{ff}^{tot} will depend on temperature down to much lower T as the correlation length ξ diverges. Thus a T dependence of S_{ff}^{tot} can be used as an initial indicator of AF order.

To determine the possibility of long-range order in the ground state, we follow the seminal analysis of Hirsch and Tang [40] in their study of the two-dimensional Hubbard model. The essence of the procedure is the observation that the correlation length $\xi(T)$ diverges as $T \rightarrow 0$, so that if one lowers T sufficiently one can satisfy the condition $\xi \gg L$: the correlation length is much larger than the linear lattice size L . The required T will, of course, decrease as L increases. If one does this for a collection of L , one has a set of measurements which is in the ground state for each L . These results can then be extrapolated to $L = \infty$ to infer the ground-state properties in the thermodynamic limit. As we shall discuss, a challenge which makes the PAM more difficult than the single band Hubbard model is the smallness of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction for weak interorbital hybridization V_{fd} , which necessitates a very large β .

Our computational approach is DQMC [41,42]. This method allows the solution of interacting tight-binding Hamiltonians like the PAM through an exact mapping onto a problem of noninteracting particles moving in a space and (imaginary) time dependent auxiliary field. This field is sampled stochastically to obtain the expectation values of different correlation functions. The update moves require the nonlocal computation of the fermion Green's function, which is also the quantity needed to measure equal time observables including the energy, double occupation, and spin correlations. The algorithm involves matrix operations and scales as the cube of the product of the number of spatial lattice sites and the number of orbitals. In certain special situations, including the PAM on the geometries studied here, the sampling is free of

the sign problem [18] so that the simulation may be conducted on large lattices (here several hundreds of spatial sites) at low temperature (here $T/t \lesssim 1/30$).

III. PAM ON THE LIEB LATTICE

We begin with the Lieb lattice which has $2N/3$ sites of coordination number $z = 2$ and $N/3$ sites with $z = 4$. Figure 4 shows $c_{ff}^{zz'}(r)$ for $V_{fd} = 0.8$ and $V_{fd} = 1.3$. In the former case, the correlation function alternates between positive and negative values, with a correlation length which exceeds the linear lattice size, as is characteristic of an AF phase. $r = 1$ corresponds to the separation between unit cells, so that integer values of r are between sites with $z' = z$ (and hence the same sublattice) and half-integer values have $z' \neq z$ (and hence occupy different sublattices). The AF correlations are evident in both $z = 2$ and $z = 4$, although they are larger for higher coordination numbers. This reflects the collective nature of the AF order, which is more robust as the number of neighbors grows. Actually, because the \mathcal{A} and \mathcal{B} sublattices have different numbers, the ordered phase is ferrimagnetic [38], with $N_\uparrow \neq N_\downarrow$ in addition to the staggered pattern seen in the figure. For $V_{fd} = 1.3$, on the other hand, $c_{ff}^{zz'}(r)$ falls rapidly to zero, indicative of a singlet phase.

The AF and singlet regimes can also be distinguished by $c_{fd}^{zz}(r=0)$, as shown in Fig. 5. (Here since $r = 0$ the coordination numbers $z' = z$.) $c_{fd}^{zz}(r=0)$ vanishes for $V_{fd} = 0$ where the localized and conduction fermions are decoupled, and saturates at a large value for $V_{fd} \rightarrow \infty$. For the sites with larger coordination number $z' = z = 4$, singlet correlations develop at larger V_{fd} than for sites with $z' = z = 2$. As might be expected for a local quantity, the singlet correlator for the $z = 4$ sites matches quite well to those on a square lattice.

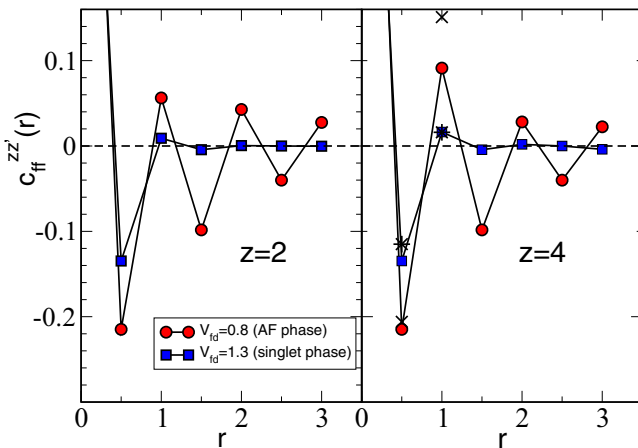


FIG. 4. Spin-spin correlation function $c_{ff}^{zz'}(r)$ as a function of r for the half-filled Lieb lattice with $U_f = 4t$ and $\beta = 30$. $r = 1$ is the unit cell size: integer r correspond to $z' = z$ and half-integer values to $z' \neq z$. The red (blue) symbols show $V_{fd} = 0.8t$ ($1.3t$), respectively. For $V_{fd} = 0.8t$ there is AF order to large r , while for $V_{fd} = 1.3$, $c_{ff}^{zz'}(r)$ decays rapidly to zero. In the AF regime, larger z increases $c_{ff}^{zz'}(r)$. Data depicted by x ($V_{fd} = 0.8$) and $*$ ($V_{fd} = 1.3$) are for the square lattice. $r = 0.5$ is for nearest-neighbors, and $r = 1.0$ for next-nearest neighbors.

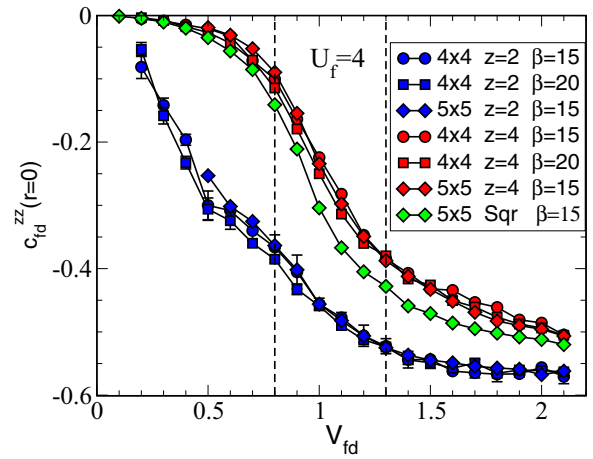


FIG. 5. Local singlet correlator $c_{fd}^{zz'}(r=0)$ for the half-filled Lieb lattice with $U_f = 4t$. The singlet correlations develop more rapidly for $z = 2$ than for $z = 4$ since for smaller coordination numbers the competition with AF order is reduced. Data for different β ($\beta = 15, 20$) as well as different system sizes (4×4 and 5×5) overlap: this short-range correlation function converges rather quickly as T is lowered and N is increased. Vertical dashed lines at $V_{fd} = 0.8, 1.3$ demark the values used for the real space spin correlation data of Fig. 4. Square lattice data coincide well with Lieb sites with $z = 4$.

(The 4×4 square lattice is anomalous because of its unusual additional symmetries, and is not shown.)

In Fig. 6 we turn to the AF structure factor, Eq. (3), which sums the spin correlations on the localized orbitals over the whole lattice. In the singlet phase, $c_{ff}^{zz'}(r)$ is short ranged and temperature independent, achieving its ground-state value at $T \sim V_{fd}^2/U_f$. In the AF phase, on the other

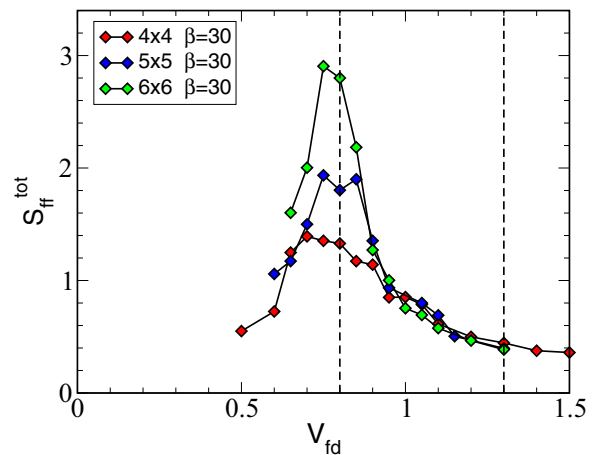


FIG. 6. Localized electron antiferromagnetic structure factor for the Lieb lattice. For $V_{fd} \gtrsim 1.1$, S_{ff}^{tot} is independent of temperature and lattice size N . However, when T is decreased for $V_{fd} \lesssim 1.1$, S_{ff}^{tot} grows as the system is cooled. These distinct behaviors reflect the completely local nature of magnetic correlations in the singlet phase, and an increasing correlation length at low T in the AF phase. Vertical dashed lines at $V_{fd} = 0.8, 1.3$ demark the values used for the real space spin correlation data of Fig. 4.

hand, the correlation length grows as T is lowered, and hence $c_{ff}^{zz'}(r)$ contributes to the structure factor out to larger and larger distances. The structure factor becomes temperature dependent at low T . These two regimes are evident, and are separated by $V_c \sim 1.1$. This is suggestive, but certainly not conclusive, evidence of the presence of a quantum critical point (QCP). At the end of the following section we will provide a finite size scaling analysis of this data to ascertain whether there is true long-range order below V_c . Note that the reduction in S_{ff}^{tot} as V_{fd} is reduced below $V_{fd} \approx 0.7$ is a finite temperature effect. The RKKY exchange scales as V_{fd}^2 and $T = t/30$ ($\beta t = 30$) is no longer low enough to reach the ground state.

IV. PAM ON A QUASICRYSTAL LATTICE

We turn now to the quasicrystal geometry. Our discussion will parallel that of the preceding section. For this lattice, the choices for coordination number are more numerous, $z = 1, 2, \dots, 8$, as evident in Fig. 2. The $z = 1, 2$ sites originate in our use of OBCs, a choice made to avoid frustration of AF order [43]. It is important to emphasize that these coordination numbers occur only at the lattice edges. Their contribution to the properties of the system will vanish in the thermodynamic limit.

$c_{ff}^{zz'}(r)$ for the quasicrystal geometry is given in Fig. 7 and shows a differentiation between long-range behavior for $V_{fd} = 0.8$ and rapid decay to zero for $V_{fd} = 1.4$. Similar to the Lieb case, $c_{ff}^{zz'}(r)$ is larger for $z = 4$ than $z = 2$. Data for other z (not shown) confirm this trend. The AF correlations extending outward from a site become more and more robust as the coordination number of the conduction orbital increases.

Figure 8 shows the singlet correlator for the $N = 239$ site quasicrystal geometry of Fig. 2 (bottom). The appearance of well-formed singlets depends on the coordination number z of the conduction electron site—the point of maximum change of

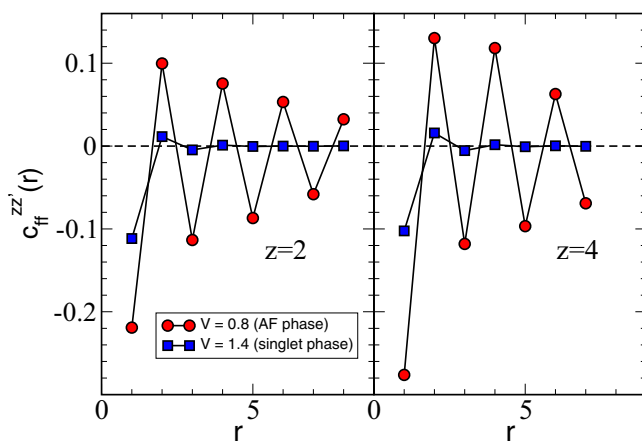


FIG. 7. z resolved spin-spin correlation function between localized orbitals for $V_{fd} = 0.8$ (AF phase) and $V_{fd} = 1.4$ (singlet phase) for the $N = 41$ quasicrystal lattice at $\beta = 30$. In the former case, $c_{ff}^z(r)$ remains nonzero out to large separations, while in the latter case it falls off to zero. Left (right) panels are $z = 2$ (4).

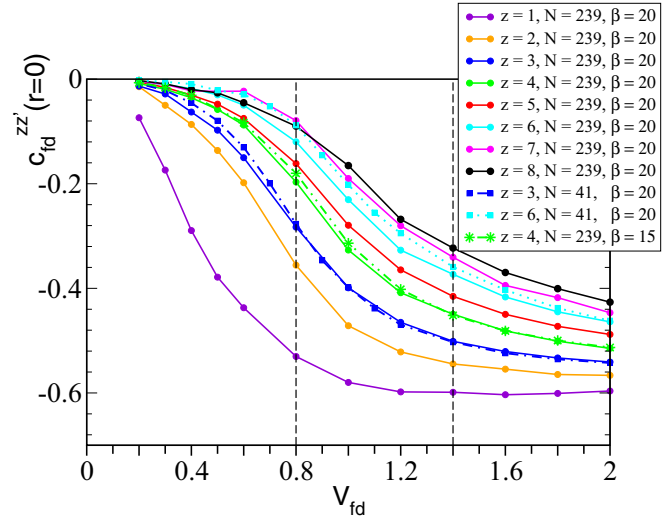


FIG. 8. The singlet correlators (circles) for the quasicrystal geometry with $N = 239$ sites and inverse temperature $\beta = 20$ shown as functions of V_{fd} . $c_{fd}^z(r=0)$ is largest in magnitude for smallest $z = 1$. The singlets become less and less well formed as z increases. Data for $N = 41$ sites (squares) indicate that finite size effects are relatively small. Similarly, data for $\beta = 15$ (diamonds) show that the low T limit has been reached. Vertical dashed lines show the V_{fd} values of Fig. 7.

$c_{fd}^{zz'}(r=0)$ shifts from $V_{fd} \sim 0.4$ to $V_{fd} \sim 1.1$ as z increases. This reflects the fact that AF is favored by a larger number of neighbors, so that the crossover to singlets requires larger V_{fd} as z increases. Since $c_{fd}^{zz'}(r=0)$ is a local quantity, its value is relatively unaffected by total lattice size (data in Fig. 8 for $N = 41$ and $N = 239$ are similar), and it also converges with β fairly quickly. (The data in Fig. 8 for $\beta = 15$ and $\beta = 20$ are similar.)

The sum of the spin-spin correlation function of localized fermions in the quasicrystal geometry yields the structure

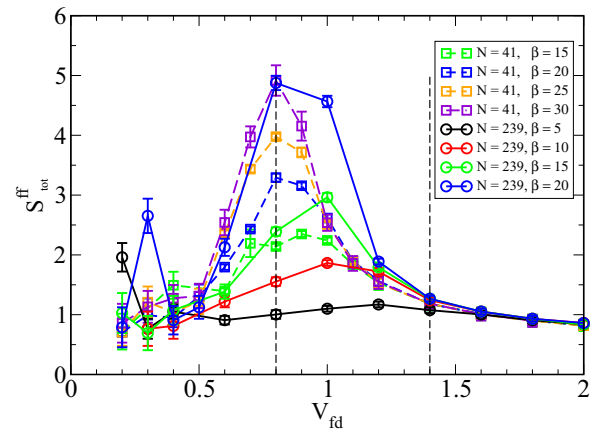


FIG. 9. S_{ff}^{tot} as a function of V_{fd} for several inverse temperatures β and quasicrystal lattice sizes $N = 41, 239$. As for the Lieb lattice, curves coincide for different β in the singlet phase at large V_{fd} , but break apart at $V_{fd} \approx 1.0-1.1$. This signals the development of antiferromagnetic correlations at large spatial separations at low V_{fd} . Vertical dashed lines show the V_{fd} values of Fig. 7.

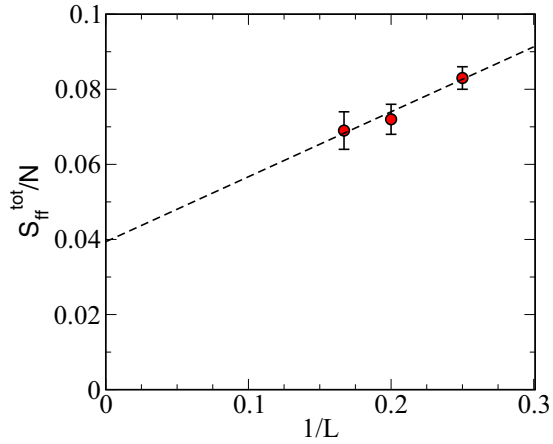


FIG. 10. Finite size scaling plot for the PAM on the Lieb lattice. Using 4×4 , 6×6 , and 8×8 unit cells, the normalized structure factor S_{ff}^{tot}/N scales to a nonzero value for $V_{fd} = 0.8$. Here the inverse temperature $\beta = 30$ which is large enough that ground-state properties have been reached for lattices of the sizes shown.

factor and is given in Fig. 9 as a function of V_{fd} . For hybridizations $V_{fd} \gtrsim 1.1$, where results in Fig. 8 suggest singlet formation is robust for all z , S_{ff}^{tot} is temperature independent. Below $V_{fd} \sim 1.1$, curves for different β break apart, suggesting that AF correlations are present and increasing as T is lowered. As noted in the discussion of Fig. 6, the reduction in the structure factor at low V_{fd} is a finite temperature effect: the effective RKKY coupling goes as V_{fd}^2 and hence even larger β is needed for AF correlations to develop at small V_{fd} (see also [44]).

In the presence of long-range order (LRO) the correlation approaches a nonzero asymptotic value $c(r \rightarrow \infty) \rightarrow m^2$, where m is the order parameter, and the structure factor scales as $S = Nm^2$. Even if LRO is present only at $T = 0$, as is the case in $d = 2$ with continuous symmetries, this scaling is observed at T low enough that the correlation length exceeds the largest linear lattice size studied. We expect $S > Nm^2$ on finite lattices, since $c(r) > m^2$ at small distances, and these short-range contributions can be substantial if the lattice size is small. A finite size scaling plot for the Lieb lattice is given in Fig. 10.

V. CONCLUSIONS

We have explored the competition between antiferromagnetic order and singlet formation in the periodic Anderson model in 2D geometries which are unfrustrated, but which have conduction electron coordination which varies from site to site. As is intuitively reasonable, singlet formation depends on z , and is delayed to larger interorbital hybridization V_{fd} as z increases. Our data suggest that, as in the case of uniform z , AF order is present in the ground state at low V_{fd} and absent at large V_{fd} . Related issues arise in models in which site dilution provides different conduction electron coordination [45,46] or in which variation in conduction electron-local orbital hybridization is considered [47].

As noted in the Introduction, the staggered moment tends to go *down* with increasing z in the spin-1/2 Heisenberg model on quasicrystal lattices [29,32–34]. Our work differs from those studies in two respects. First, we consider itinerant, rather than localized spins. Second, we consider a model with two moments per site, one associated with the conduction electron band and one with the local band. It is not completely clear which of these differences is responsible for the alteration in the effect of local z on the spin correlations. It might be of interest to study a single band (Hubbard) model with variable z to isolate the answer to this question. A number of experimental systems also exhibit a similar behavior in which $T_{\text{Néel}}$ can be higher at the (lower z) surface than in the (higher z) bulk [48]. Our work, and much of the literature, has considered models with variable z which, however, remain bipartite. The combined of frustration and variable z are studied in [35].

Both geometries studied have unusual $U_f = 0$ single-particle eigenstates. In the case of the Lieb lattice, the inequivalence of the number of sites in the A and B sublattices leads to the presence of flatbands. In the true quasicrystal geometry (of which we explore only an approximant) the eigenstates exhibit an intermediate scaling with system size, between the limits where the participation ratio \mathcal{P} grows with the number of sites, as occurs for Bloch states, and $\mathcal{P} \sim o(1)$ for conventional localization [23,27]. Thus our work also explores the effects of those features of the noninteracting spectrum on magnetic correlations in the presence of interactions.

Limitations on accessible system sizes and temperatures prevent us from addressing high-precision questions such as whether the distribution of z destroys a sharp QCP between the AF and singlet phases and replaces it with a more gradual crossover. Related dynamical mean-field theory work [27] indicates that there is a range of Kondo temperatures. It is interesting to note that, to within the accuracy DQMC simulations provide, there is remarkably little variation between the critical value of V_{fd} for different 2D conduction electron geometry. The QCP appears to be quite close to the square lattice value $V_{fd}/t \approx 1$ for the Lieb and quasicrystal lattices considered here.

The usual view of the PAM is of a two-band (conduction and localized) tight-binding Hamiltonian. Although we have emphasized here the presence of sites with different conduction electron lattice coordination numbers, an alternate perspective on our work is that of a study of a PAM in which the conduction electrons themselves have several bands. The Lieb lattice geometry, for example, has three sites per unit cell, and hence three conduction bands (Fig. 3), in addition to the localized orbitals. Our DQMC simulations indicate that the competition between singlet formation and AF order is not fundamentally affected by this more complex band structure.

ACKNOWLEDGMENTS

The work of N.H. was supported by NSF-PHY-1263201 (REU program). R.T.S. and W.-T.C. were supported by Grant No. DE-SC0014671. We are grateful to E. Andrade and V. Dobrosavljevic for useful conversations.

- [1] M. Rasetti, *The Hubbard Model—Recent Results* (World Scientific, Singapore, 1991).
- [2] *The Hubbard Model*, edited by Arianna Montorsi (World Scientific, Singapore, 1992).
- [3] F. Gebhard, *The Mott Metal-Insulator Transition, Models and Methods* (Springer, New York, 1997).
- [4] P. Fazekas, *Lecture Notes on Electron Correlation and Magnetism* (World Scientific, Singapore, 1999).
- [5] P. W. Anderson, Localized magnetic states in metals, *Phys. Rev.* **124**, 41 (1961).
- [6] S. Doniach, The Kondo lattice and weak antiferromagnetism, *Physica B+C* **91**, 231 (1977); B. Cornut and B. Coqblin, Influence of the crystalline field on the Kondo effect of alloys and compounds with Cerium impurities, *Phys. Rev. B* **5**, 4541 (1972).
- [7] J. Kondo, Theory of Dilute Magnetic Alloys, *Solid State Phys.* **23**, 183 (1970).
- [8] M. A. Ruderman and C. Kittel, Indirect exchange coupling of nuclear magnetic moments by conduction electrons, *Phys. Rev.* **96**, 99 (1954).
- [9] T. Kasuya, A Theory of Metallic Ferro- and Antiferromagnetism on Zener's Model, *Prog. Theor. Phys.* **16**, 45 (1956).
- [10] K. Yosida, Magnetic properties of Cu-Mn Alloys, *Phys. Rev.* **106**, 893 (1957).
- [11] C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963).
- [12] G. R. Stewart, Heavy-fermion systems, *Rev. Mod. Phys.* **56**, 755 (1984).
- [13] G. R. Stewart, Non-Fermi-liquid behavior in d- and f-electron metals, *Rev. Mod. Phys.* **73**, 797 (2001).
- [14] R. Blankenbecler, J. R. Fulco, W. Gill, and D. J. Scalapino, Ground-state properties of the periodic Anderson model, *Phys. Rev. Lett.* **58**, 411 (1987).
- [15] R. M. Fye, Quantum Monte Carlo study of the one-dimensional symmetric Anderson lattice, *Phys. Rev. B* **41**, 2490 (1990).
- [16] M. Vekic, J. W. Cannon, D. J. Scalapino, R. T. Scalettar, and R. L. Sugar, Competition between Antiferromagnetic Order and Spin-Liquid Behavior in the Two-Dimensional Periodic Anderson Model at Half Filling, *Phys. Rev. Lett.* **74**, 2367 (1995).
- [17] C. Huscroft, A. K. McMahan, and R. T. Scalettar, Magnetic and Thermodynamic Properties of the Three-Dimensional Periodic Anderson Hamiltonian, *Phys. Rev. Lett.* **82**, 2342 (1999).
- [18] E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, Sign problem in the numerical simulation of many-electron systems, *Phys. Rev. B* **41**, 9301 (1990).
- [19] Matthias Troyer and Uwe-Jens Wiese, Computational Complexity and Fundamental Limitations to Fermionic Quantum Monte Carlo Simulations, *Phys. Rev. Lett.* **94**, 170201 (2005).
- [20] M. Jarrell, H. Akhlaghpour, and T. Pruschke, Periodic Anderson Model in Infinite Dimensions, *Phys. Rev. Lett.* **70**, 1670 (1993).
- [21] K. Held, C. Huscroft, R. T. Scalettar, and A. K. McMahan, Similarities between the Hubbard and Periodic Anderson Models at Finite Temperatures, *Phys. Rev. Lett.* **85**, 373 (2000).
- [22] S. Nakatsuji, S. Yeo, L. Balicas, Z. Fisk, P. Schlottmann, P. G. Pagliuso, N. O. Moreno, J. L. Sarrao, and J. D. Thompson, Intersite Coupling Effects in a Kondo Lattice, *Phys. Rev. Lett.* **89**, 106402 (2002).
- [23] S. Seo, X. Lu, J.-X. Zhu, R. R. Urbano, N. Curro, E. D. Bauer, V. A. Sidorov, L. D. Pham, T. Park, Z. Fisk, and J. D. Thompson, Disorder in quantum critical superconductors, *Nat. Phys.* **10**, 120 (2014).
- [24] K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura, and T. Ishimasa, Quantum critical state in a magnetic quasicrystal, *Nat. Mater.* **11**, 1013 (2012).
- [25] T. Watanuki, S. Kashimoto, D. Kawana, T. Yamazaki, A. Machida, Y. Tanaka, and T. J. Sato, Intermediate-valence icosahedral Au-Al-Yb quasicrystal, *Phys. Rev. B* **86**, 094201 (2012).
- [26] N. J. Curro, Nuclear magnetic resonance in the heavy fermion superconductors, *Rep. Prog. Phys.* **72**, 026502 (2009).
- [27] E. C. Andrade, A. Jagannathan, E. Miranda, M. Vojta, and V. Dobrosavljevic, Non-Fermi-Liquid Behavior in Metallic Quasicrystals with Local Magnetic Moments, *Phys. Rev. Lett.* **115**, 036403 (2015).
- [28] U. W. Grimm and M. Schreiber, in *Quasicrystals—Structure and Physical Properties*, edited by H.-R. Trebin (Wiley-VCH, Weinheim, 2003), pp. 210–235.
- [29] A. Jagannathan and F. Piéchon, Energy levels and their correlations in quasicrystals, *Philos. Mag.* **87**, 2389 (2006).
- [30] A quasicrystal approximant is a periodic crystal whose atomic arrangement shares the local structure of the quasicrystal. See A. I. Goldman and R. F. Kelton, Quasicrystals and crystalline approximants, *Rev. Mod. Phys.* **65**, 213 (1993).
- [31] A. Jagannathan, Quantum Spins and Quasiperiodicity: A Real Space Renormalization Group Approach, *Phys. Rev. Lett.* **92**, 047202 (2004).
- [32] S. Wessel, A. Jagannathan, and S. Haas, Quantum Antiferromagnetism in Quasicrystals, *Phys. Rev. Lett.* **90**, 177205 (2003).
- [33] S. Wessel and I. Milat, Quantum fluctuations and excitations in antiferromagnetic quasicrystals, *Phys. Rev. B* **71**, 104427 (2005).
- [34] A. Jagannathan, R. Moessner, and Stefan Wessel, Inhomogeneous quantum antiferromagnetism on periodic lattices, *Phys. Rev. B* **74**, 184410 (2006).
- [35] D. J. J. Farnell, O. Götze, J. Richter, R. F. Bishop, and P. H. Y. Li, Quantum $s = 1/2$ antiferromagnets on Archimedean lattices: The route from semiclassical magnetic order to nonmagnetic quantum states, *Phys. Rev. B* **89**, 184407 (2014).
- [36] Stefanie Thiem and J. T. Chalker, Long-range magnetic order in models for rare-earth quasicrystals, *Phys. Rev. B* **92**, 224409 (2015).
- [37] E. Y. Vedmedenko, U. Grimm, and R. Wiesendanger, Non-collinear Magnetic Order in Quasicrystals, *Phys. Rev. Lett.* **93**, 076407 (2004).
- [38] E. H. Lieb, Two Theorems on the Hubbard Model, *Phys. Rev. Lett.* **62**, 1201 (1989).
- [39] One could, of course, also separate the spin correlations based on the coordination number z' of the site $i + r$. In the case of the Lieb lattice, where there are only two pairs of choices $z, z' = 1, 2$ this would be feasible, but in the case of the quasicrystal geometry where $z, z' = 1, 2, \dots, 8$ such a refined breakdown would probably do more to obscure the analysis of the physics than to clarify it.
- [40] J. E. Hirsch and S. Tang, Antiferromagnetism in the Two-Dimensional Hubbard Model, *Phys. Rev. Lett.* **62**, 591 (1989).
- [41] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Monte Carlo calculations of coupled boson-fermion systems. I, *Phys. Rev. D* **24**, 2278 (1981).

- [42] J. E. Hirsch, Two-dimensional Hubbard model: Numerical simulation study, *Phys. Rev. B* **31**, 4403 (1985).
- [43] PBCs are usually employed to reduce finite size effects and give a more rapid approach to the thermodynamic limit, since they eliminate special features like reduced coordination number of sites at the lattice boundary. In the quasicrystal lattice, which has a distribution of z even in the absence of OBCs, it is less clear that PBCs are to be preferred. Furthermore, frustration which would be introduced by the use of PBCs would cause the formation of domain walls which would have a similar large finite size effect as OBCs.
- [44] T. Paiva, G. Esirgen, R. T. Scalettar, C. Huscroft, and A. K. McMahan, Doping-dependent study of the periodic Anderson model in three dimensions, *Phys. Rev. B* **68**, 195111 (2003).
- [45] A. W. Sandvik, Quantum Criticality and Percolation in Dimer-Diluted Two-Dimensional Antiferromagnets, *Phys. Rev. Lett.* **96**, 207201 (2006).
- [46] Kaj H. Höglund, A. W. Sandvik, and S. Sachdev, Impurity Induced Spin Texture in Quantum Critical 2D Antiferromagnets, *Phys. Rev. Lett.* **98**, 087203 (2007).
- [47] A. H. Castro Neto, G. Castilla, and B. A. Jones, Non-Fermi Liquid Behavior and Griffiths Phase in f-Electron Compounds, *Phys. Rev. Lett.* **81**, 3531 (1998).
- [48] F. Zhang, S. Thevuthasan, R. T. Scalettar, R. R. P. Singh, and C. S. Fadley, Monte Carlo study of magnetic order at ferromagnetic and antiferromagnetic surfaces: Implications for spin-polarized photoelectron diffraction, *Phys. Rev. B* **51**, 12468 (1995).