Magnetic Correlations in a Periodic Anderson Model with Non-Uniform Conduction Electron Coordination

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The Periodic Anderson Model (PAM) is widely studied to understand strong correlation physics and especially the competition of antiferromagnetism and singlet formation. Quantum Monte Carlo (QMC) studies have focused both on issues such as the nature of screening and locating the quantum critical point (QCP) at zero temperature and also on possible experimental connections to phenomena ranging from the Cerium volume collapse to the relation of the magnetic susceptibility and Knight shift in heavy fermions. In this paper we extend QMC work to lattices in which the conduction electron sites can have variable coordination. This situation is relevant both to recently discovered magnetic quasicrystals and also to magnetism in doped heavy fermion systems.

PACS numbers: 71.10.Fd, 71.30.+h, 02.70.Uu

INTRODUCTION

The single band Hubbard Hamiltonian\textsuperscript{1–4} captures several of the most fundamental consequences of electron-electron interactions in solids, namely magnetic order and the Mott metal-insulator transition. Although the question is still open, it may even contain the several of the most fundamental consequences of electron--electron interactions in solids, namely magnetic order and the Mott metal-insulator transition. Although the question is still open, it may even contain the singlet formation\textsuperscript{9}, when the conduction and localized electrons are strongly hybridized, and ordering of the local moments mediated indirectly through the Ruderman-Kittel-Kasuya-Yosida interaction\textsuperscript{11–13}.

In heavy fermion materials\textsuperscript{14, 15}, this competition is believed to explain different low temperature phases, e.g. non-magnetic CeAl\textsubscript{3} where the \( f \) moments are screened by the conduction electrons, and CeAl\textsubscript{2} which becomes antiferromagnetic (AF) at low temperatures. Likewise, in Ce metal itself, as well as in other rare-earths, the tuning of the \( f-d \) hybridization \( V_{fd} \) through pressure is believed to play a crucial role in the ‘volume collapse’ transition\textsuperscript{16–21}.

Quantum Monte Carlo (QMC) studies of the PAM have explored some of this physics, in one\textsuperscript{22, 23}, two\textsuperscript{24}, and three dimensions\textsuperscript{25}. 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\textsuperscript{26, 27}. QMC in infinite dimensions\textsuperscript{28} 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\textsuperscript{29}. Another motivation is provided by chemical substitution in heavy fermion materials, either by the replacement of some of the local moment atoms by non-magnetic ones, as in (Ce,La)CoIn\textsubscript{5}\textsuperscript{30} or by changes to the conduction orbitals, as in the alloying of Cd onto In sites in CeCo(In,Cd)\textsubscript{5}\textsuperscript{31, 32}. 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\textsuperscript{33, 34}. In these Au-Al-Yb alloys (Au\textsubscript{51}Al\textsubscript{34}Yb\textsubscript{15}), measurements of the magnetic susceptibility \( \chi \) and specific heat \( C \) diverge as \( T \to 0 \). 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 resonances\textsuperscript{35}.

The NFL behavior of Au-Al-Yb alloys has recently been studied by solving the \( U = \infty \) Anderson Impurity Model (AIM) for a single local moment coupled to conduction electrons in a quasicrystal approximant geometry\textsuperscript{36}. The crucial result is that singular responses in \( \chi \) 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 2D “Ammann-Beenker” tiling\textsuperscript{37, 38}. Quasicrystalline approximants\textsuperscript{39} for Au\textsubscript{51}Al\textsubscript{34}Yb\textsubscript{15} are in 3D; the quasi-periodic 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 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 non-uniform. Our work extends that of [30] by examining a dense array of local orbitals and also by including the effect of finite $U_t$. 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 [32].

The magnetic properties of quantum antiferromagnets in geometries which have variable coordination number (the crown, dice, and CaVO lattices) have also been studied in the context of the spin-1/2 Heisenberg Hamiltonian [40-42]. Surprisingly, unlike the case of regular geometries where the ordered moment increases from the honeycomb ($z = 3$) to square ($z = 4$) lattices, it is found that the local AF order parameter decreases with $z$. We will comment on this further in our conclusions.

**MODEL AND METHODS**

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

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} (d_{i \sigma}^{\dagger} d_{j \sigma} + d_{j \sigma}^{\dagger} d_{i \sigma}) - V_{fd} \sum_{i \sigma} (d_{i \sigma}^{\dagger} f_{i \sigma} + f_{i \sigma}^{\dagger} d_{i \sigma}) + U_t \sum_{i} (n_{i \uparrow} - \frac{1}{2})(n_{i \downarrow} - \frac{1}{2})$$

Here $t$ is the hybridization between conduction orbitals with creation/destruction operators $d_{i \sigma}^{\dagger}$ ($d_{i \sigma}$) on near neighbor sites $\langle ij \rangle$. In this paper we consider the two conduction electron geometries shown in Figs. [12] corresponding to “Lieb” and “quasicrystal” lattices respectively. Each site of these lattices also contains a localized orbital, creation/destruction operators $f_{i \sigma}^{\dagger}$ ($f_{i \sigma}$), $U_t$ 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. [12] 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 $t, U_t, V_{fd}$. Half-filling optimizes the tendency for AF correlations, and also allows DQMC simulations at low temperature since the sign problem [26] is absent.

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 [43] 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 non-interacting 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 $U_t/t \gtrsim 4$ are insensitive to the presence of a $U_t/t = 0$ band gap [29].

![Figure 1](image.png)

**FIG. 1**: (Color online) The Lieb lattice geometry under consideration in this paper. (Cluster shown has 4x4 unit cells with 48 sites). Each site contains both a conduction ($d$) orbital and a localized ($f$) orbital, so that there is a total of 96 sites/orbitals. Lines correspond to the $d$-$d$ hopping $t$, with eight possible coordinations $z = 1, 2, \cdots, 8$. We use periodic boundary conditions (pbc). 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 $V_{fd}$.

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

$$c_{ii}^{zz}(r) = \langle f_{i+\hat{r},\downarrow} f_{i,\uparrow} f_{i,\uparrow}^{\dagger} f_{i+\hat{r},\downarrow}^{\dagger} \rangle$$
$$c_{dd}^{zz}(r) = \langle d_{i+\hat{r},\downarrow} d_{i,\uparrow} d_{i,\uparrow}^{\dagger} d_{i+\hat{r},\downarrow}^{\dagger} \rangle$$
$$c_{fd}^{zz}(r) = \langle f_{i,\uparrow}^{\dagger} d_{i,\uparrow} d_{i,\uparrow}^{\dagger} f_{i+\hat{r},\downarrow} \rangle$$

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 [44]. We focus here on $c_{ii}^{zz}(r)$ which measures intersite magnetic correlations between the local electrons, and $c_{dd}^{zz}(r = 0)$, 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,
FIG. 2: (Color online) Top (bottom): Approximants to the Au$_{51}$Al$_{134}$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. 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 (OBC) 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. but depend more generally on both $i$ and $r$ in irregular lattices.

We also measure the structure factor,

$$S^z_{ll} = \sum_{i} \sum_{i'} c^{z'}_i (r) (-1)^r$$

$$S^{\text{tot}}_{ll} = \sum_r \sum_{z,z'} g^{zz'} c^{z'}_i (r) (-1)^r \tag{3}$$

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 $\pm 1$ on the two sublattices of the bipartite geometry and hence measures AF order. The $z$-resolved contributions to the total structure factor $S^{\text{tot}}_{ll}$ 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 $S^{\text{tot}}_{ll}$ 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, $S^{\text{tot}}_{ll}$ will depend on temperature down to much lower $T$ as the correlation length $\xi$ diverges. Thus a $T$ dependence of $S^{\text{tot}}_{ll}$ can be used as an indicator of AF order.

FIG. 3: (Color online) 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 $\delta$ 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 [36, 42].
Our computational approach is determinant Quantum Monte Carlo (DQMC). This method allows the solution of interacting tight-binding Hamiltonians like the PAM through an exact mapping onto a problem of non-interacting 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 non-local computation of the fermion Green’s function, which 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 so that the simulation may be conducted on large lattices (here several hundreds of spatial sites) at low temperature (here \( T/t \lesssim 1/30 \)).

**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 \( c_{zz'}^{\pm}(r) \) for \( V_{Id} = 0.8 \) and \( V_{Id} = 1.3 \). 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 number. This reflects the collective nature of the AF order, which is more robust as the number of neighbors grows. Actually, because the \( A \) and \( B \) sublattices have different numbers, the ordered phase is Ferrimagnetic, with \( N_A \neq N_B \) in addition to the staggered pattern seen in the Figure. For \( V_{Id} = 1.3 \), on the other hand, \( c_{zz'}^{\pm}(r) \) falls rapidly to zero, indicative of a singlet phase.

The AF and singlet regimes can also be distinguished by \( c_{zz'}^{\pm}(r = 0) \), as shown in Fig. 5. (Here since \( r = 0 \) the coordination numbers \( z' = z \).) \( c_{zz}^{\pm}(r = 0) \) vanishes for \( V_{Id} = 0 \) where the localized and conduction fermions are decoupled, and saturates at a large value for \( V_{Id} \rightarrow \infty \). For the sites with larger coordination number \( z' = 4 \), 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. (The \( 4 \times 4 \) 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, \( c_{zz'}^{\pm}(r) \) is short ranged and temperature independent, achieving its ground state value at \( T \sim V_{Id}^2/U_1 \). In the AF phase, on the other hand, the correlation length grows as \( T \) is lowered, and hence \( c_{zz'}^{\pm}(r) \) 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 \( V_{c} \approx 1.1 \). This is suggestive, but certainly not conclusive, evidence of the presence of a 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 \( S_{Bz}^{npt} \) 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.

**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, $z = 1, 2, \cdots 8$, as evident in Fig. 2. The $z = 1, 2$ sites originate in our use of OBC, a choice made to avoid frustration of AF order[47]. 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.

$c^{zz'}_f(r)$ for the quasi-crystal 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, $c^{zz'}_f(r)$ 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 $c^{zz}_f(r = 0)$ 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 cross-over to singlets requires larger $V_{fd}$ as $z$ increases. Since $c^{zz}_f(r = 0)$ 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 $\beta$ fairly quickly. (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 quasi-crystal geometry yields the structure factor and is given in Fig. 9 as a function of $V_{fd}$. For hybridizations $V_{fd} \gtrsim 1.1$, $S_{ht}^{tot}$ is independent of temperature and lattice size $N$. However, when $T$ is decreased for $V_{fd} \lesssim 1.1$, $S_{ht}^{tot}$ 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.

In the presence of long range order (LRO) the correlation approaches a nonzero asymptotic value $c(r \to \infty) \to m^2$, where $m$ is the order parameter, and the structure factor scales as $S = N m^2$. Even if LRO is present only at $T = 0$, as is the cases 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 $S > N m^2$ 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 is given in Fig. 10.

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 orbital 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 \cite{49,50} or in which variation in conduction electron-local orbital hybridization is considered \cite{51}. It is interesting to note that the anomalous tendency for the staggered moment to go down with increasing $z$ in the spin-1/2 Heisenberg model on quasicrystal lattices \cite{38,40,42} would be even more evident in itinerant Hamiltonians such as that studied here, since the greater coordination number reduces the local moment. A number of experimental systems also exhibit a similar behavior in which $T_{Neel}$ can be higher at the (lower $z$) surface than in the (higher $z$) bulk.\cite{52}

Both geometries studied have unusual $U_t = 0$ single

![Figure 7](image_url)

**FIG. 7:** (Color online) $z$ 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, $c^z_{fd}(r)$ remains non-zero out to large separations, while in the latter case it falls off to zero. Left(right) panels are $z = 2(4)$.

![Figure 8](image_url)

**FIG. 8:** (Color online) The singlet correlators (circles) for the quasicrystal geometry with $N = 239$ sites and inverse temperature $\beta = 20$ shown as functions of $V_{fd}$. $c^z_{fd}(r = 0)$ 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.

![Figure 9](image_url)

**FIG. 9:** (Color online) $S^z_{tot}$ as a function of $V_{fd}$ for several inverse temperatures $\beta$ and quasicrystal lattice sizes $N = 41, 239$. As for the Lieb lattice, curves coincide for different $\beta$ 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: (Color online) Finite size scaling plot for the PAM on the Lieb lattice. Using 4x4, 6x6, and 8x8 unit cells, the normalized structure factor $S_{\text{tot}}^N/N$ 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.

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.

ACKNOWLEDGEMENTS

The work of NH was supported by NSF-PHY-1263201 (REU program). RTS and WTC were supported by [de- sc0014671]. We are grateful to Eric Andrade and Vladimir Dobrosavljevic for useful conversations.

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[47] PBC 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 OBC, it is less clear that PBC are to be preferred. Furthermore, frustration which would be introduced by the use of PBC would cause the formation of domain walls which would have a similar large finite size effect as OBC.

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