We demonstrate the existence of ferromagnetism in the Periodic Anderson Model (PAM) at conduction-band filling near a quarter. We show that this ferromagnetism is not supported by Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions but is instead driven by the precursors of charge density wave (CDW) formation in the conduction electron band. To study the effect of spatial correlations, we compare Dynamical Mean field Approximation (DMFA) and Dynamical Cluster Approximation (DCA) results. We find that both RKKY and CDW driven ferromagnetism persist as short-range correlations are incorporated into the theory. Both DMFA and DCA show the precursors of CDW formation through the strong enhancement of the d-electron CDW susceptibility as the temperature decreases, up to the ferromagnetic transition temperature. In addition, the DCA captures the signal of a band gap opening due to Peierls instability.

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Rare-earth and actinide-based heavy fermion (HF) systems display a wide variety of interesting phenomena, including Kondo insulator, fermi and non-fermi liquid paramagnetism, ferromagnetism, antiferromagnetism and superconductivity [1]. Among these phenomena, ferromagnetism is especially interesting since while a number of HF ferromagnetic compounds exist [2], few experimental studies on the ferromagnetic phase diagrams are available [3]. Although a number of theoretical studies of HF ferromagnetism are available [4, 5, 6, 7, 8, 9, 10, 11, 12, 13], the range of ferromagnetism in the local moment regime has not been fully clarified, and the mechanisms leading to ferromagnetic order are still not well understood.

In this Letter, we investigate charge density wave (CDW) driven ferromagnetism occurring near a quantum critical point (QCP) around quarter filling of the conduction band in the Kondo regime of the Periodic Anderson Model (PAM). The ferromagnetism in the region of low conduction band filling (e.g. \( n_d \approx 0.5 \)) is attributed to the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction between the f-electron local moments mediated by the conduction (d-) electrons [4, 5, 6, 7, 8, 10, 11, 12, 13]. Whereas at \( n_d \approx 1 \) the RKKY and superexchange interactions lead to antiferromagnetic order [14, 15]. However, in the region near quarter filling \( n_d \approx 0.5 \), close to a QCP associated with a vanishing ferromagnetic transition temperature, the mechanism leading to magnetic order is not well understood. We provide theoretical evidence arising from the incorporation of spatial correlations into the theory that the ordering near quarter filling of the conduction band in the PAM is enhanced by CDW fluctuations. Previous studies (e.g. [8] and [11]) likely did not find ferromagnetic ordering at this filling due to the difficulty of capturing strong CDW correlations with earlier methods.

Our interest is enhanced by the discovery of the ferromagnetic superconductor UGe2 [16], where superconductivity coexists with ferromagnetism near its ferromagnetic QCP. Pressure-dependence studies indicate that there may be different mechanisms driving the ferromagnetic order in this material [17, 18]. One scenario suggests that the superconducting-ferromagnetic coexistence is related to coupled charge and spin density waves [19]. Although our model is not detailed enough to describe Uranium-based compounds, our results suggest that a CDW mechanism might play an important role in driving the ferromagnetic order near the QCP in UGe2.

As briefly mentioned in a previous study of the infinite dimensional PAM [14], Kondo screening plays an important role in triggering the ferromagnetism when the RKKY and superexchange interactions favor antiferromagnetism. We refer to this as charge density wave (CDW) driven ferromagnetism, since the alignment of the f-electron local moments is caused by coherent Kondo screening induced by the conduction electrons forming a CDW. Fig. 1 illustrates this process. Imagine there are roughly \( N/2 \) localized (f) electrons and \( N/4 \) itinerant (d) electrons in the system, where \( N \) is the number of lattice sites. At some low temperature each d electron locally screens one f electron through antiferromagnetic alignment of their spins. These local screening clouds [20, 21] become larger at lower temperatures. As a result, the \( N/4 \) d electrons tend to screen all \( N/2 \) f electrons coherently. This process requires that the d electrons form a spin-polarized CDW, since in order to maximize kinetic energy gain and maintain the coherent Kondo screening a d electron must hop to nearest neighbor sites with unoccupied d orbitals.

Formalism. Since Dynamical Mean Field Theory (DMFT) [22] in infinite dimensions has a local self energy, questions arise as to whether the CDW ferromagnetic mechanism persists in a finite dimensional system and how spatial correlations may affect the results. In this Letter, we present our study on the three-dimensional PAM using the Dynamical Cluster Approximation (DCA) [23]. We find that the CDW driven fer-
romagnetism persists as short-range spatial correlations are incorporated into the theory. In addition, we present one and two-particle evidence of the precursors of CDW formation to support this ferromagnetic mechanism.

The PAM Hamiltonian can be written as

\[
H = -t \sum_{\langle i,j \rangle \sigma} (d_i^{\dagger}d_j + h.c.) + \sum_{i \sigma} (\epsilon_d d_i^{\dagger}d_i + \epsilon_f f_i^{\dagger}f_i) + V \sum_{i \sigma} (d_i^{\dagger}f_i + h.c.) + \sum_i U(n_{f\uparrow} - 1/2)(n_{f\downarrow} - 1/2),
\]

where \(d(f)^{(i)}\) destroys(creates) a \(d(f)\) electron at site \(i\) with spin \(\sigma\), \(t\) is the nearest-neighbor \(d\)-electron hopping, \(\epsilon_d\) and \(\epsilon_f\) the orbital energy of the \(d\) and \(f\) electrons respectively, \(V\) the \(d-f\) hybridization, and \(U\) the on-site Coulomb repulsion between \(f\) electrons. In this Hamiltonian we set the chemical potential to zero.

We work with a simple cubic lattice with bare conduction band-width \(W = 12t\) and \(V = W/3\) to satisfy the Zlatić-Horvatić criterion for the strong-coupling regime [21]: \(u = U/\Gamma > 2\), where \(\Gamma = V^2 N(0)\) and \(N(0)\) is the bare conduction band density of states at the Fermi level. The Hirsch-Fye Quantum Monte Carlo (QMC) algorithm [27] is used to solve the DCA cluster problem. We perform calculations for two different cluster sizes: \(N_c = 1\), equivalent to DMFA, and \(N_c = 14\). We choose the bipartite cluster 14A, which is considered the first “good” cluster with \(N_c > 1\), following the selection criterion of Betts [27, 28]. Following the procedure in Ref. [14], for every \(n_d\) value, we choose \(\epsilon_d - \epsilon_f\) such that \(n_f \approx 1\) at a moderate temperature, say \(\beta = 1/10\), and keep the value of \(\epsilon_d - \epsilon_f\) fixed as the temperature is decreased. The values of \(\epsilon_d\) and \(\epsilon_f\) are adjusted (keeping \(\epsilon_d - \epsilon_f\) fixed) during the self-consistent iterations to satisfy \(n_f \approx 1\) and the chosen value of \(n_d\). To study the systematic errors associated with the imaginary time increment \((\Delta \tau)\) in the QMC we compare the results with \(\Delta \tau = 1/4\) and \(\Delta \tau = 1/16\).

Results. The upper panel of Fig. 2 shows the FM Curie temperature, \(T_c\), versus \(n_d\), with \(T_c\) vanishing at \(n_d\) slightly higher than 0.6. Comparison between results for \(N_c = 1\) with \(\Delta \tau = 1/4\) and \(\Delta \tau = 1/16\) suggests that \(\Delta \tau = 1/4\) is sufficient to capture the correct profile of the phase diagram. Comparison between results for \(N_c = 1\) and \(N_c = 14\) with the same \(\Delta \tau = 1/4\) indicates that spatial correlations decrease \(T_c\), as generally expected [23]. The lower panel of Fig. 2 shows the dependence of \(\Delta J_{RKKY}\) on \(n_d\). Here \(\Delta J_{RKKY}\) is defined as \(\Delta J_{RKKY} = J_{AFM}^{RKKY} - J_{FM}^{RKKY}\), with \(J_{AFM}^{RKKY} = J_{RKKY}(q = (\pi, \pi, \pi))\) and \(J_{FM}^{RKKY} = J_{RKKY}(q = (0, 0, 0))\), so that a negative (positive) \(\Delta J_{RKKY}\) signals a ferromagnetic (antiferromagnetic) RKKY coupling between neighboring local moments. We define \(J_{RKKY}(q) \approx -2J_{fd}T\sum_k N(k, \omega_n)G(k, \omega_n)G(k + q, \omega_n)\), with \(J_{fd} \approx 8V^2/\Gamma\), as in Ref. [14]. For both \(N_c = 1\) and \(N_c = 14\), we take \(\Delta \tau = 1/4\), and show that for three different temperatures close to \(T_c\) (\(T_c = 1/60, 1/70\), and \(1/80\)) there is no significant difference in \(\Delta J_{RKKY}\). It is clear that for both values of \(N_c\) the RKKY coupling changes from ferromagnetic to antiferromagnetic in a region where the phase is still ferromagnetic. In this region, where \(\Delta J_{RKKY} > 0\), ferromagnetism can not be explained by the RKKY mechanism. Note that the region of ferromagnetism supported by the RKKY mechanism becomes wider as \(N_c\) changed from 1 to 14. Since, for a given \(n_d\), RKKY coupling favors ferromagnetic alignment when the magnitude of the Fermi vector satisfies \(k_F < \pi/4\), this result suggests that the Fermi surface shrinks as spatial correlations are introduced.

To address the mechanism of ferromagnetic order in the region of the phase diagram where RKKY interactions favor antiferromagnetism, we provide evidence that in this region ferromagnetism is driven by the precursors of charge density wave formation. In support of this
idea, Fig. 3 shows that at low temperatures the d-electron CDW susceptibility, $\chi_{CDW} \equiv \chi_{\text{charge}}(\mathbf{q} = (\pi, \pi, \pi))$, is strongly enhanced relative to the ‘bulk’ (uniform) charge susceptibility, $\chi_{\text{Bulk}} \equiv \chi_{\text{charge}}(\mathbf{q} = (0, 0, 0))$, for $n_d$ values corresponding to the ferromagnetic phase region not supported by the RKKY mechanism. Based on geometry one expects the CDW configuration be best achieved when $n_d = 0.5$, which implies that $\chi_{CDW}$ would be most strongly enhanced for $n_d = 0.5$. However, our results show that the maximum enhancement occurs around $n_d \approx 0.55$, which may, again, indicate shrinking of the Fermi surface. In the inset of Fig. 3 we plot $\chi_{CDW}$ versus $T$ for $n_d = 0.4$, 0.5, and 0.6, showing its enhancement at low temperatures. In these calculations, $t\Delta T = 1/4$. For smaller values of $t\Delta T$ (not shown), $\chi_{CDW}$ increases, but the peak location does not shift.

To elaborate further on how the CDW driven ferromagnetism works, note that, as shown in the inset of Fig. 3, $\chi_{CDW}$ reaches a maximum at temperatures around $T \approx 1/40 - 1/60$, and decreases slightly when the temperature is lowered close to $T_c$. The non-local correlations enhance $\chi_{CDW}$, and we also find that they enhance the screened local moment for $n_d \approx 0.5$, while they suppress it at other fillings (not shown). This may be interpreted as an attempt to balance the kinetic and potential energies of the Kondo lattice. The system can optimize the exchange energy by localizing a d electron in a singlet with the f moment on half the sites. This is balanced by the kinetic energy in the usual way by allowing the d electrons to delocalize and screen other f-electron local moments forming Kondo ‘clouds’. However, when $n_d \approx 0.5$, the system may gain additional kinetic energy though the gap that accompanies a d-electron charge density wave (CDW). Note that this is not a well-defined CDW phase, since such an ordering would be manifest in the divergence of $\chi_{CDW}$, and a full gap would suppress Kondo screening. As the temperature is lowered further, the local Kondo screening clouds grow, so that the overlap between the Kondo clouds drive the d electrons to collaborate to screen the f electrons coherently. In doing so, each d electron forms a Kondo singlet with an f electron at a site only momentarily, then hops to one of its neighboring sites to regain the resonance with the f electron at that site. This process forces the f-electron local moments to align, hence the system forms a ferromagnetic phase. The momentary breaking of the Kondo singlet due to hopping of the d electrons to their neighboring sites decreases their staggered charge correlation. Thus, this explains why $\chi_{CDW}$ is suppressed slightly as the temperature approaches $T_c$.

So far we have shown that DMFA can already capture the d-electron CDW precursors at the two-particle level, i.e. in the $\chi_{CDW}$ behavior. In the following, we show that by incorporating the spatial correlations within DCA ($N_c > 1$), the CDW precursors can also be captured at the one-particle level, e.g. through the d-electron density of states (DOS). In order to capture the effective modulation potential inducing the Peierls instability [29], the self energy must have sufficiently strong k dependence. This is only possible for $N_c \gg 1$. When this modulation potential is properly captured by the self energy, the corresponding d-electron DOS forms a gap or signals of a gap opening, such as a “dip”, around the chemical potential. In our model, the chemical potential is set fixed to zero, but we adjust $\epsilon_d$ to satisfy the desired filling. Therefore, if a gap or a “dip” occurs in the DOS, it should be manifest in a plot of $\epsilon_d$ versus $n_d$. Fig. 3 shows how the $\epsilon_d$ vs $n_d$ profile evolves from high to low temperatures for $N_c = 1$ and $N_c = 14$. It is clear that for $N_c = 14$ (right panel), but not for $N_c = 1$ (left panel), the $\epsilon_d$ vs $n_d$ curve bends slightly near $n_d \approx 0.5 - 0.55$ at $T \approx 1/40$, which coincides with the strongest enhancement in $\chi_{CDW}$. We interpret this as the signal of a gap opening accompanying the formation of a CDW in the d-electron DOS. As the temperature is lowered further, e.g. from $T \approx 1/40$ to $T \approx 1/70$, the bending in the $\epsilon_d$ vs $n_d$ curve does not become more prominent, and diminishes as the temperature becomes closer to $T_c$, e.g. $T \approx 1/90$ (not shown). This indicates that the gap never fully opens, and the d-electron DOS increases back as the d electrons become more mobile to screen coherently at temperatures closer to $T_c$.

Our arguments may be justified also by inspection of the Kondo screening length [20, 21] and its consistency with the $\chi_{CDW}$ and the d-electron density of states as discussed before. The magnitude of the Kondo coupling in our system is $J_{fd} \approx 8\gamma^2/U \approx 0.6W \approx 7t$. According to the scaling theory of Sorensen et al. [20], this coupling strength roughly corresponds to the Kondo screening length, $\xi_L$, of the order of a lattice constant or less. This is consistent with our picture of localized Kondo ‘clouds’ when the CDW forms. This screening length depends on the d-electron density of states at the chemical

![Figure 3](image-url)
FIG. 4: Comparing $\varepsilon_d$ versus $n_d$ for $N_c = 14$ and $N_c = 1$. For $N_c = 14$ (right panel) bending in the $\varepsilon_d$ vs $n_d$ curve is observed, indicating the tendency to the formation of a band gap due to Peierls' instability. This feature is not seen for $N_c = 1$ (left panel).

potential, $\rho(0)$, through $\xi_L \propto \exp[-1/\rho(0)J_f d]$. Since $\rho(0)$ increases as the temperature approaches $T_c$ (as discussed in the previous paragraph), the screening length also increases accordingly. In turn, the overlap between screening clouds enables the $d$ electrons to mediate ferromagnetic coupling between $f$-electron local moments.

**Conclusion.** We have shown that the ferromagnetism in the strong coupling regime of the PAM has two mechanisms. In the region of low conduction band filling ferromagnetism is driven by the RKKY exchange interaction, while in the region of higher conduction band fillings up to slightly more than a quarter the precursors of a CDW formation in the $d$ electrons induce the magnetic order. We have demonstrated that the CDW formation can be captured within the DMFA and DCA through the enhancement of $d$-electron CDW susceptibility. In addition, the DCA captures the signal of a band gap opening due to the Peierls instability that drives the CDW formation.

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