Similarities between the Hubbard and Periodic Anderson Models at Finite Temperatures

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The single band Hubbard and the two band Periodic Anderson Hamiltonians have traditionally been applied to rather different physical problems - the Mott transition and itinerant magnetism, and Kondo singlet formation and scattering off localized magnetic states, respectively. In this paper, we compare the magnetic and charge correlations, and spectral functions, of the two systems. We show quantitatively that they exhibit remarkably similar behavior, including a nearly identical topology of the finite temperature phase diagrams at half-filling. We address potential implications of this for theories of the rare earth “volume collapse” transition.

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The single band Hubbard model (HM) and the two band Periodic Anderson model (PAM) have a long history in the study of many body effects in solids. While they have been proposed to describe complex d- and f-electron systems, respectively, the detailed atomic physics and orbital structure are nevertheless eliminated, leaving minimal Hamiltonians where the interplay between electron kinetic energy, screened electron-electron repulsion, the Pauli principle, temperature, and electron density still give rise to a rich variety of phenomena.

The key features of the half-filled HM are antiferromagnetism and a Mott insulator-metal transition within the paramagnetic phase. Originally, the Mott transition was associated with a change in the density of states (DOS) from widely separated upper and lower Hubbard bands to a broad one-peak structure, and an accompanying loss of local moments. The key features of the PAM are magnetism arising from an indirect ‘RKKY’ interaction of the three local moments mediated by the conduction electrons, and a DOS which, in the paramagnetic phase, has a three peak structure - upper and lower bands and an additional Abrikosov-Suhl resonance near the Fermi surface. Concomitant with the development of this resonance, local moments become screened by the conduction electrons, and an anomalous sharp feature in the free energy is observed. During the past years, it has been established by dynamical mean-field theory (DMFT) and quantum Monte Carlo (QMC) simulations that the HM also has a three peak structure in its paramagnetic DOS, thereby blurring at least one of the features believed to distinguish the two models.

It is the purpose of this paper to note even greater similarity between the two models at finite temperature, especially if a more physical choice is taken for the interband hybridization in the PAM. Specifically, our new DMFT results show that the f-electrons of the PAM undergo a transition similar to the Mott transition of the HM, as is reflected by the f-electron spectral function, quasiparticle weight, and charge compressibility. Furthermore, the phase diagrams, at finite temperature, associated with the two models are topologically equivalent.

These similarities are of particular interest in that the HM and PAM (or its impurity approximation) have been proposed as competing models for the “volume-collapse” transitions in the rare earth and actinide metals. These pressure-induced phase transitions are characterized by unusually large (9–15%) volume changes, and are believed to arise from f-electron correlation effects. The present paper suggests that the predictions of the two models are more similar than has previously been thought, and that perceived incompatibilities may have arisen in part from differing and less rigorous approximations used in the treatment of electron correlations, as for example in mean-field-like local-density functional theory.

The single band HM is given by,

\[ H = \sum_{k\sigma} \epsilon_k f_{k\sigma}^\dagger f_{k\sigma} + U_f \sum_i (n_{if\uparrow} - \frac{1}{2})(n_{if\downarrow} - \frac{1}{2}). \]  

Here \( \epsilon_k^f = \epsilon_0^f - 2t_{df}(\cos(k_x) + \cos(k_y) + \cos(k_z)) \) is the nearest-neighbor band dispersion, where the energy scale is set by \( t_{ff} = 1 \), and \( U_f \) is the f-electron local interaction on every lattice site \( i \). The two band PAM is,

\[ H = \sum_{k\sigma} [\epsilon_k^d d_{k\sigma}^\dagger d_{k\sigma} + \epsilon_k^f f_{k\sigma}^\dagger f_{k\sigma} + V_k (d_{k\sigma}^\dagger f_{k\sigma} + h.c.)] + U_f \sum_i (n_{if\uparrow} - \frac{1}{2})(n_{if\downarrow} - \frac{1}{2}), \]

where \( V_k \) denotes the hybridization between f and d electrons at momentum \( k \). In the PAM, the d-electrons are chosen to have the same nearest-neighbor dispersion as the f-electrons of the HM (\( t_{dd} = 1 \)), while the f-electrons are chosen to be dispersionless, \( t_{ff} = 0 \). We study the
“symmetric” PAM, i.e., $c_0^{d(f)} = 0$ and chemical potential $\mu = 0$, which has the property that $\langle n_f \rangle = \langle n_d \rangle = 1$ for all choices of $U_f$, $t_{dd(f)}$, $t_{fd}$, and temperature $T$. Finally, we choose a nearest-neighbor intersite hybridization $V_{k} = -2t_{fd} \cos(k_{x}) + \cos(k_{y}) + \cos(k_{z})$, but also have investigated the more canonical onsite hybridization $V_{k} = \sqrt{3}t_{fd}$, as well as an odd-parity nearest-neighbor form $V_{k} = -it_{fd} \sin(k_x) + \sin(k_y) + \sin(k_z)$. The three choices have zero, constant, and maximal $|V_{k}|$ on the half-filled Fermi surface, respectively; and yield metallic, insulating, and semi-metallic $f$-projected densities of states, respectively, at $U = 0$ and within a Fermi liquid phase.

We favor intersite $V_{k}$ due to the similarity of its metallic $f$-DOS to paramagnetic local density results for the rare earths and to the character of their $f$-electrons the high pressure phases. However, it is to be emphasized that the essential results of this paper are independent of these hybridization choices.

Our calculational approaches are dynamical mean-field theory (DMFT) [13,14], and determinant quantum Monte Carlo (QMC) [13,14], carried out for a three-dimensional simple-cubic lattice in the thermodynamic limit and for a 4$^3$ periodic lattice, respectively. DMFT can capture thermodynamic phase transitions while the quantitative agreement with QMC provides compelling evidence its accuracy.

Within DMFT, both the $f$-electron part of the PAM and the HM map onto the same single site problem in which the Green function is calculated from a dynamical mean field $\Sigma_{f}(\omega)$ [3,15]. The difference between PAM and HM is the way $\epsilon_{k}^{f}$ and $V_{k}$ enter the self-consistency condition, i.e., the $k$ integrated Dyson equation

$$G_{f}(\omega) = \frac{1}{(2\pi)^{3}} \int d^{3}k \frac{1}{\omega - \Sigma(\omega) - \epsilon_{k}^{f} - V_{k}^{2}/(\omega - \epsilon_{k}^{d})}.$$  \hspace{1cm} (3)

where $V_{k} = 0$ and $\epsilon_{k}^{d} = 0$ for the HM and PAM, respectively. In the DMFT equations the $d$-electrons of the PAM, which enter only quadratically, have been integrated out yielding an effective $f$-electron problem with retarded potential $V_{k}^{2}/(\omega - \epsilon_{k}^{d})$. One expects the different potentials to be reflected in quite distinct physical properties of the two models.

The spectral function $A_{f}(\omega)$ of the $f$-electrons is shown in Fig.1. At small hybridizations $t_{fd}$, the PAM spectrum consists of two peaks at $\pm U/2$ which corresponds to a phase with localized $f$-electrons. At larger $t_{fd}$, an additional Abrikosov-Suhl resonance develops at the Fermi energy which is not gapped for the PAM with intersite hybridization. Thus, the $f$-electrons are itinerant. The striking similarity to the spectral function of the HM (inset) calls for a more quantitative comparison of the crossover between itinerant and localized $f$-electrons which is driven by an increase of $U_{f}/t_{fd(f)}$. Such a detailed comparison is the subject of this paper.

![FIG. 1.](image_url) The spectral function of the PAM at $U_{f} = 6$ and $T = 0.2$ with an intersite hybridization of (a) $t_{fd} = 0.3$ and (b) $t_{fd} = 1$, respectively, as obtained by DMFT (solid line) and QMC (dashed line). With the exception of a small AF splitting of the central resonance found in finite-d simulations at $t_{fd} = 1$ the agreement between DMFT and QMC is excellent. Insets: HM (DMFT) at $U_{f} = 6$, $T = 0.2$, $\tau_{ff} = 0.3$ and $t_{ff} = 1$, respectively.

In the self energy $\Sigma_{f}$ (Fig.2a), the crossover [10] shows up as an abrupt change of the behavior with $t_{fd}$: for large $t_{fd}$ Fermi liquid behavior with $\text{Im} \Sigma_{f}(i\omega_{n}) \propto \omega_{n}$ at low (Matsubara) frequencies occurs, while at small $t_{fd}$ an insulating-like behavior with diverging $\text{Im} \Sigma_{f}$ is observed. From the $\Sigma_{f}$ data one can calculate a quantitative measure for the crossover from itinerant to localized $f$-electrons: the quasiparticle weight of the Abrikosov-Suhl resonance $Z_{f} = (1 - \partial \Sigma_{f}(\omega)/\partial \omega|_{\omega=\omega_{n}})^{-1}$ (calculated via finite differential quotient $1 - \text{Im} \Sigma_{f}(\omega_{n})/\omega_{n}$). Just as at the Mott transition of the HM (Fig.1b), $Z_{f}$ vanishes with decreasing $t_{fd}/U_{f}$ for the PAM. This behavior of the PAM is astonishingly similar to that seen in the HM and is insensitive to the choice of hybridization as is seen in Fig. 2b.

While the important similarity between the two models lies in the presence or absence of the central resonance as a whole (measured by $Z_{f}$), the PAM hybridization can determine finer details such as whether this resonance may be split by a gap. Consider the charge compressibility $\kappa_{f} = \partial n_{f}/\partial \mu$ shown in Fig. 2c. Nonzero $\kappa_{f}$ indicates a metallic phase, while $\kappa_{f}$ is exponentially small in $1/T$ within a gapped insulating phase. At small $t_{fd(f)}$, all $f$ spectral functions show insulating behavior as there are no central resonances lying between the two

FIG. 1. The spectral function of the PAM at $U_{f} = 6$ and $T = 0.2$ with an intersite hybridization of (a) $t_{fd} = 0.3$ and (b) $t_{fd} = 1$, respectively, as obtained by DMFT (solid line) and QMC (dashed line). With the exception of a small AF splitting of the central resonance found in finite-d simulations at $t_{fd} = 1$ the agreement between DMFT and QMC is excellent. Insets: HM (DMFT) at $U_{f} = 6$, $T = 0.2$, $\tau_{ff} = 0.3$ and $t_{ff} = 1$, respectively.
Hubbard bands. These resonances form in all cases at larger $t_{fd(fft)}$, however, they are split by insulating and semimetallic hybridization gaps for the onsite and odd-parity cases, respectively, as is evident in Fig. 2c.

The behavior for the HM (not shown) is very similar. (b) Quasiparticle weight $Z_f$ as a function of $t = t_{fd}$ and $t = t_{ff}$ for the PAM and HM, respectively ($\square$: PAM with intersite, $\Delta$: PAM with onsite, and $\triangledown$: PAM with odd-parity intersite hybridization; $\blacksquare$: HM). (c) Electronic compressibility $\kappa_f = \partial \bar{n}_f / \partial \mu$ as a function of $t$. All results are calculated by DMFT at $U_f = 6$ and $T = 0.15$ ($\Delta, \triangledown$: $T = 0.07$).

While the (unscreened) local moment $\langle m_z^2 \rangle = \langle (n_\uparrow - n_\downarrow)^2 \rangle$ shown in Fig. 3 decreases with increasing hybridization, it is still quite substantial through the HM and PAM crossovers of Fig. 2, marked by arrows in Fig. 3. This smooth behavior of the local moment from weak to strong coupling in both models is insufficiently appreciated in the discussions of the distinctions between the 'Mott' and 'Kondo' scenarios for the volume collapse transition, where mean field treatments of the correlations lead to artificially abrupt changes in the local moment. Despite the finite moments, screening effects lead to Pauli like low-T susceptibilities at large $t_{fd(fft)}$.

FIG. 3. The square of the local moment is shown as a function of $t = t_{fd}$ and $t = t_{ff}$ for the PAM with intersite hybridization (open symbols) and HM (closed symbols), respectively, at $U_f = 6$ and $T = 0.15$ (circles: DMFT, squares: QMC) [$T = 0.5$ for the QMC HM to avoid antiferromagnetic ordering]. In neither case does the moment change remarkably in the vicinity of the transitions of Fig. 2 (arrows).

The $T$-$U_f$ phase diagrams which result from consideration of the self-energy, quasiparticle weight, and magnetic susceptibility are shown in Fig. 4. Both the HM and PAM have a low temperature phase of antiferromagnetic order with a maximum in the Néel temperature $T_N$ at intermediate $U_f/W$. At a slightly larger $U_f/W$, a second transition, i.e., the disappearance of the quasiparticle peak, is observed within the paramagnetic phase (if antiferromagnetism is frustrated). This is the Mott transition of the HM and, from the Kondo point of view, the crossing of the Kondo temperature $T_K(t_{fd})$. Apart from the temperature and hybridization scales, the phase diagrams of HM and PAM are remarkably similar at finite $T$. It is an open question at present whether such similarities will persist down to zero temperature.

The present paper has shown a remarkable similarity between the HM and the f-electron system of the PAM which is indeed – after integrating out the d-electrons – like a HM with a more complicated retarded potential. Novel numerical results on the spectral functions, charge compressibilities and local moments show that despite its more complicated potential, the PAM undergoes (at finite temperatures and half-filling) a crossover from itinerant to localized f-electrons similar to the Mott transition of the HM. While this similarity is closest for the PAM with intersite hybridization which describes metallic f-electrons at large $t_{fd}$ the vanishing of the central resonance does not depend on the hybridization choice. This crossover and the transition towards antiferromagnetic order yield phase diagrams which have the same topology for both models. Accordingly, the present paper suggests that the physics underlying the Mott [8]
not transitions in f-electron metals [10,11] may be similar and 
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FIG. 4.  \( T-U_f \) phase diagram of the Hubbard model with 
a semi elliptic DOS (filled symbols; reproduced from [20,18]) 
and PAM with intersite hybridization (open symbols) within 
DMFT. Here \( W \) is the band width of the Bethe DOS and 
12 \( t_{fd} \) for the PAM, respectively. Squares: Néel temperature; 
triangles: Mott transition/Kondo temperature (the dashed 
lines end at higher \( T \) as the crossover becomes too gradual in 
\( U_f/W \) to allow a precise location). 

(HM) and the Kondo volume collapse scenarios [8] (PAM 
or its impurity approximation) for the volume collapse 
transitions in f-electron metals [10,11] may be similar and 
not incompatible. While the Mott transition is continuous 
at the temperatures considered, the rapid change in the 
correlation energy, when combined with the smooth 
contributions from other valence bands, might nevertheless 
result in a Maxwell construction giving the thermo-
dynamic instability manifested as the first-order vol-
ume collapse in Ce [21]. 

In regard to local density calculations, orbitally-
polarized and self-interaction-corrected applications [22] 
to the volume-collapse transitions resemble a mean field 
solution of the HM, where the transition coincides with a 
coalescence of the two Hubbard bands and a simultane-
ous loss of local moment. The implication of the present 
paper is that regardless of the balance between f-f (HM) 
and f-valence hybridization (PAM), a correlated solution 
should show some Kondo-like attributes in the collapsed 
phase, including an analog of the three-peak local DOS, 
persistence of the local moment, and its screening as de-
duced from the susceptibility. Local density theory does 
not show such Kondo-like features in the collapsed phase, 
however, it does nevertheless yield excellent structural-
dependence of the total energy [23]. 

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