Gutzwiller approximation for inter-orbital spin-triplet pairing in multi-band Anderson lattice model

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Motivation

The explanation of the nature of the superconducting phases coexistent with ferromagnetism, found in several uranium-based heavy-fermion compounds, poses a challenge to theorists [1]. Recently, a satisfactory model of the magnetism in UGe_2 was proposed [2]. Previously, it was shown that Hund's exchange J can drive spin-triplet superconductivity in Hubbard-type multi-band models [3]. Here we extend the model for UGe_2 by introducing doubly degenerate bands and J in order to investigate whether it admits spin-triplet orbital-singlet s-wave solutions for the superconducting gap.

Model and method

We investigate a doubly degenerate (2 conduction c and 2 f electron bands) extended periodic Anderson model on the 2D square lattice:

$$H = \sum_{\mathbf{ij}l\sigma} t_{\mathbf{ij}l} c^\dagger_{\mathbf{i}l\sigma} c_{\mathbf{j}l\sigma} + \epsilon_f \sum_{\mathbf{i}l\sigma} f^\dagger_{\mathbf{i}l\sigma} f_{\mathbf{i}l\sigma} + V \sum_{\mathbf{i}l\sigma} \left(f^\dagger_{\mathbf{i}l\sigma} c_{\mathbf{i}l\sigma} + \text{h.c.} \right)$$
$$+ U \sum_{\mathbf{i}l} n^f_{\mathbf{i}l\uparrow} n^f_{\mathbf{i}l\downarrow} - 2J \sum_{\mathbf{i}} \left(\mathbf{S}^f_{\mathbf{i}1} \mathbf{S}^f_{\mathbf{i}2} + \frac{1}{4} n^f_{\mathbf{i}1} n^f_{\mathbf{i}2} \right)$$
$$+ (U - 2J) \sum_{\mathbf{i}\sigma\sigma'} n^f_{\mathbf{i}1\sigma} n^f_{\mathbf{i}2\sigma'} + J \sum_{\mathbf{i}} \left(f^\dagger_{\mathbf{i}1\uparrow} f^\dagger_{\mathbf{i}1\downarrow} f_{\mathbf{i}2\downarrow} f_{\mathbf{i}2\uparrow} + \text{h.c.} \right).$$

We apply the multi-band Gutzwiller approximation as developed by Bünemann and Gebhard (cf. [3, 4] and references therein), which is a variational method within which evaluation of observables is exact in $d = \infty$ limit. We present the values of the following (variational) quantities obtained as a result of the optimization procedure

$$n_f = 2 \sum_\sigma \langle n^f_{\mathbf{i}l\sigma} \rangle, \quad m_f = \left(\langle n^f_{\mathbf{i}l\uparrow} \rangle - \langle n^f_{\mathbf{i}l\downarrow} \rangle \right), \quad A_{f\sigma} = \langle f_{\mathbf{i}1\sigma} f_{\mathbf{i}2\sigma} \rangle.$$

In the procedure, we fix the total band-filling $n = \sum_{l\sigma} \langle n^f_{\mathbf{i}l\sigma} + n^c_{\mathbf{i}l\sigma} \rangle$. The essence of Gutzwiller approximation is renormalization of bare model parameters. Thus, we also present the renormalization factor of the hybridization term

$$Q_\sigma = \frac{V_{\sigma,\text{eff}}}{V} = \frac{1}{V} \frac{\partial \langle H \rangle}{\partial \langle f^\dagger_{\mathbf{i}l\sigma} c_{\mathbf{i}l\sigma} \rangle}.$$

Conclusions

- Our model and approximation lead to spin-triplet orbital-singlet s-wave pairing among minority spin electrons (A1 phase) within the strong (FM2) and the weak ferromagnetic (FM1) phases.
- In the paramagnetic phase (PM) spin-triplet pairing amplitude $A_{f\sigma}$ does not vanish and is equal in both spin channels (A phase).
- The highest pairing amplitude $A_{f\downarrow}$ occurs at the transition point between FM2 and FM1.
- The results may serve as a starting point for the explanation of the origin of superconductivity in UGe_2.

References

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Acknowledgement

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Ground state result

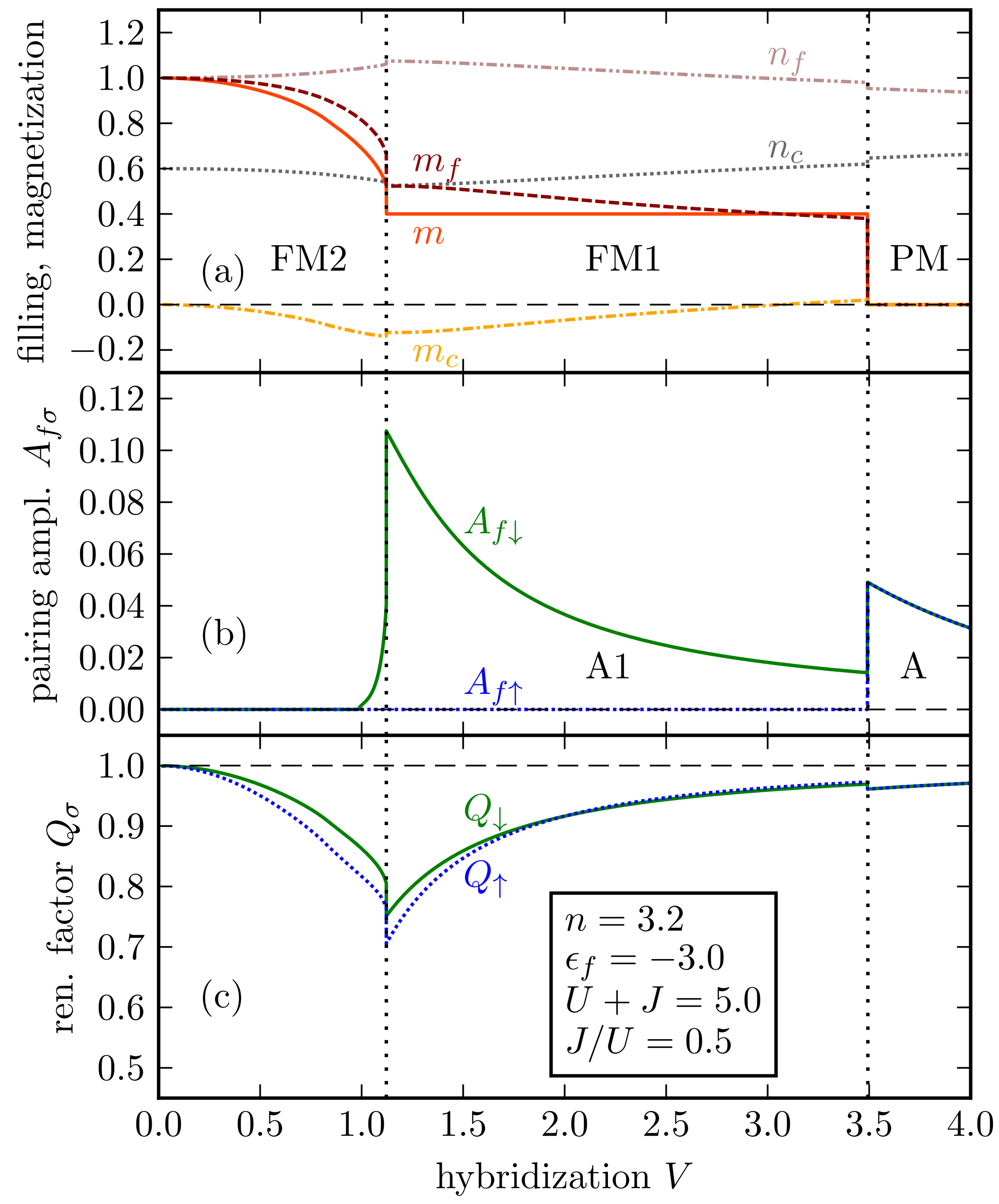

Figure 1: (a) Fillings and magnetizations of c and f states, and the total magnetization $m = m_f + m_c$, (b) pairing amplitudes $A_{f\sigma}$, (c) renormalization factors Q_σ, all as functions of hybridization V for square lattice density of c states: t=-1 (n.n.), t'=0.25 (n.n.n.)

J dependence of results

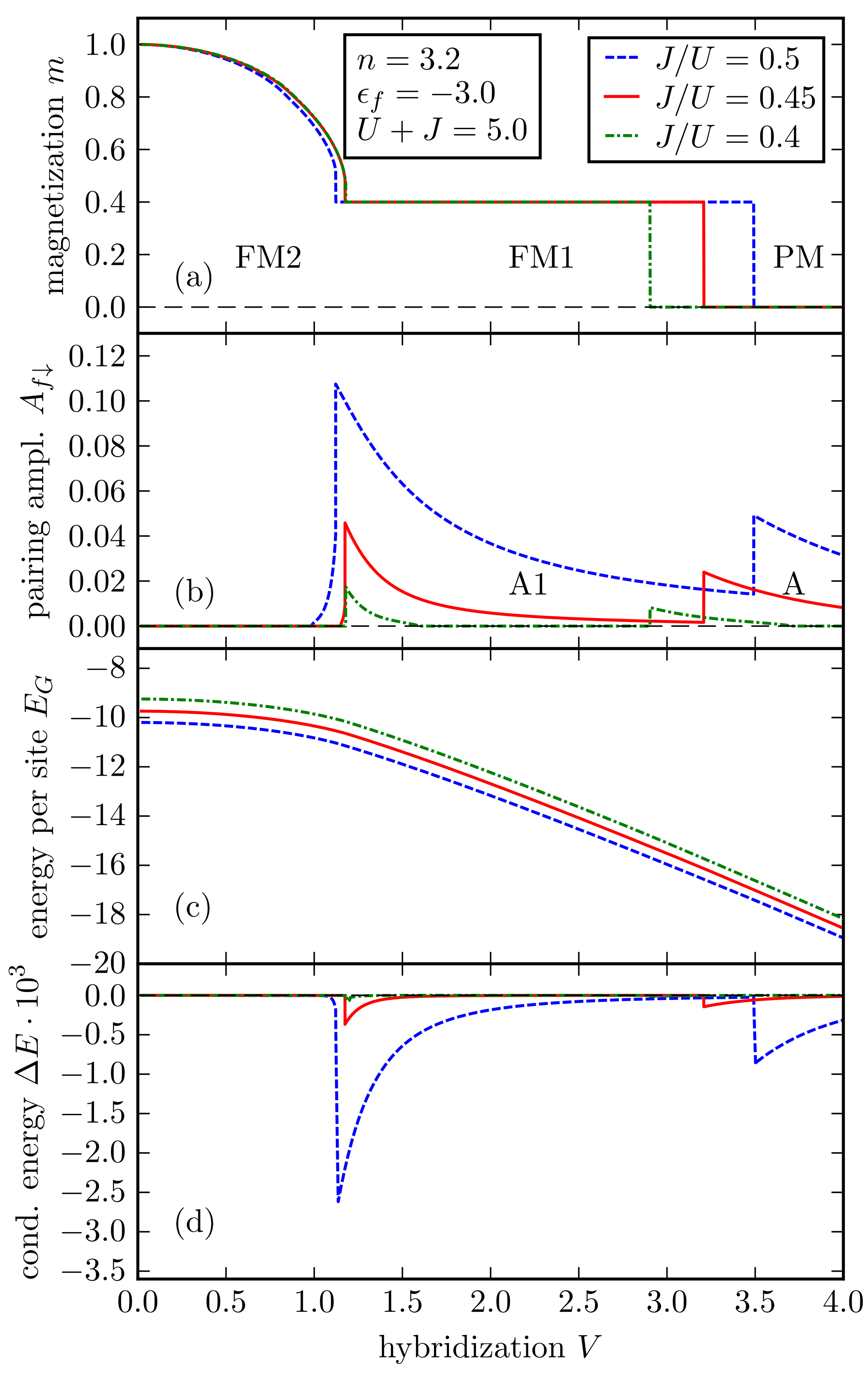

Figure 2: (a) The total magnetization m, (b) pairing amplitude $A_{f\downarrow}$, (c) ground state energy per lattice site $E_G = \langle H \rangle / N$, (d) superconducting condensation energy $\Delta E = E_G(\text{normal}) - E_G(\text{SC})$. In A1 phase $A_{f\uparrow}$=0, while in A phase $A_{f\uparrow}$=$A_{f\downarrow}$.