Comment on "Theory of Unconventional Spin Density Wave: A Possible Mechanism of the Micromagnetism in U-based Heavy Fermion Compounds"

In the recent Letter [1] a new, very attractive idea is proposed for the explanation of the micromagnetism in U-based heavy fermion (HF) compounds. For this sake a nontrivial spin density wave (SDW) state is introduced in the framework of the Hamiltonian:

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - 2J \sum_{\langle ij \rangle} \vec{S}_i \vec{S}_j + \left(V - \frac{J}{2} \right) \sum_{\langle ij \rangle \sigma \sigma'} n_{i,\sigma} n_{j,\sigma'}, \quad (1)$$

where we used the same notations as in [1] except $\vec{S}_i = \frac{1}{2} c_i^\dagger \vec{\sigma} c_i$. Unlike the conventional SDW, the order parameter $\Psi_k^Q \equiv \sum_\sigma \sigma \langle c_{k\sigma}^\dagger c_{k+Q\sigma} \rangle$ in the unconventional SDW (d-SDW) [1] state is characterized by "d-wavelike" k dependence $\Psi_k^Q \propto \cos k_x - \cos k_y$ [2]. In this case the ordered staggered magnetic moment M_Q is equal to zero. The authors restricted themselves to a very special case of 2D electron system in a simple square lattice, the shape of the Fermi surface corresponding to the *perfect nesting* with $Q = (\pi, \pi)$. The direct and exchange interaction constants are chosen positive $V > 0$, $J > 0$ [3].

We are not going to discuss the origin of the model (1) and criticize its applicability to the essentially 3D HF compounds (such as UPt_3 and URu_2Si_2 [4]) without any experimental evidence of perfect or imperfect nesting. Our goal is to claim, that even in the model considered in [1], the mean-field (MF) analysis performed by the authors is incomplete and the phase diagram obtained (see Fig. 1 in [1]) is wrong.

To begin with, let us look carefully on the Hamiltonian (1). One can easily see that this Hamiltonian contains the Coulomb interaction and the *ferromagnetic* [3] exchange integral. Thus, there are at least four ordered states which may be realized in this model: itinerant ferromagnet (FM) state, conventional SDW, charge density wave (CDW), and d-SDW. One can expect that the FM state, missed by [1], will be dominant at least in the limit $U, V \ll J$. Therefore, to construct a complete phase diagram, the FM state should also be incorporated into the MF approach.

Let us consider first the case $(U, V, J) \ll t$ when the nesting property is important and MF analysis is reasonable. The criterion of instability can be determined from the behavior of the static response functions [5]: $\chi_\alpha(q,0) = \chi_\alpha^0(q,0)/[1 - I_\alpha(q)\chi_\alpha^0(q,0)]$, where $\alpha = \mathrm{FM}, \mathrm{DW}$, $I_{\mathrm{FM}}(0) = U + 4J$, $I_{\mathrm{SDW}}(Q) = U - 4J$, $I_{\mathrm{CDW}}(Q) = 8V - U - 4J$, and $I_{d\text{-SDW}}(Q) = V$. For the perfect nesting case $\chi_{\mathrm{DW}}^0(Q,0) \sim (1/t)\log^2(t/T)$ [6], where one power of logarithm comes from nesting and another one is due to the Van Hove singularity (VHS). Nevertheless, $\chi_{\mathrm{FM}}^0(0,0) \sim (1/t)\log(t/T)$ is also singular [6] due to VHS. The MF critical temperatures [7] are $T_{\mathrm{DW}}^{\mathrm{MF}} \sim t\exp(-2\pi\lambda_{\mathrm{DW}}\sqrt{t/I_{\mathrm{DW}}})$ and $T_{\mathrm{FM}}^{\mathrm{MF}} \sim t\exp(-2\pi\lambda_{\mathrm{FM}} t/I_{\mathrm{FM}})$, $\lambda_\alpha \sim 1$. Thus, the FM state certainly wins when $J \gg (U, V)$ and $V/J \lesssim J/t$ and even overcomes d-SDW in the phase diagram (Fig. 1 in [1]). The SDW state is more favorable when $U \gg (V, J)$ and the CDW state occurs when $V \gg (U, J)$. We also emphasize that unlike VHS, an additional "nesting" singularity in $\chi(Q,0)$ is very sensible to a variety of effects, such as interlayer tunneling, doping, next hopping, etc., making the application of model [1] to real systems nearly impossible.

Let us consider another important limit $U \gg (t, V, J)$, the most realistic one, since the one-site U should be larger than the other nearest-neighbor interactions V, J and $t \sim m_*^{-1} \ll t_0$ ($m_* \gg m_0$ is an effective HF mass, m_0 and t_0 correspond to noninteracting fermions). In this case the V term is irrelevant for the half-filled band due to the constrain $n_i = 1$, nesting is not important, and only the AF state with $I_{\mathrm{AF}} \sim t^2/U$ [8] is possible (when $J/t < t/U$).

To conclude, the new d-SDW state predicted in [1] cannot be realized for the most physically reasonable limits. The phase diagram in [1] is wrong, resulting in an erroneous statement of the d-SDW stability region. The very narrow region of parameters U, V, J, t (which has nothing to do with those presented in [1]) where the d-SDW state may exist requires a more detailed analysis.

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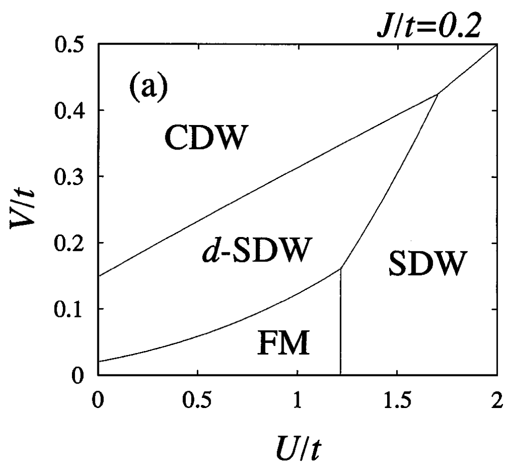
[1] H. Ikeda and Y. Ohashi, Phys. Rev. Lett. **81**, 3723 (1998).
[2] d-SDW is more favorable among all other SDW (extended s and p states) due to the Van Hove singularity.
[3] There is not any unconventional SDW state for $J \leq 0$.
[4] N. Grewe and F. Steglich, in *Handbook of the Physics and Chemistry of Rare Earths*, edited by K. A. Gschneider, Jr. and L. Eyring (Elsevier, Amsterdam, 1991), Vol. 14, p. 343.
[5] For simplicity, we use the random phase approximation.
[6] J. E. Hirsh, Phys. Rev. B **31**, 4403 (1985).
[7] There is no true transition to a state with long range order in a 2D system with a continuous symmetry except for $T = 0$.
[8] P. W. Anderson, Phys. Rev. **115**, 2 (1959).

Ikeda and Ohashi Reply: In our previous Letter [1], we proposed an unconventional spin density wave state as a possible mechanism of the micromagnetism in URu_2Si_2. As an example, we studied the d-wave spin density wave (d-SDW). This novel SDW can explain various experimental results. Kiselev and Bouis [2] (KB) have pointed out that the ferromagnetic (FM) state should be considered in the phase diagram (Fig. 1 in [1]) and the d-SDW cannot be realized for the most physically reasonable limits.

In [1], we analyzed the simplest model for the d-SDW [Eq. (1) in [1]] within the mean field theory. It was implicitly assumed that the antiferromagnetic state in URu_2Si_2 originates from the nesting in the heavy fermion state [3]. Then, among the possible orderings, we examined only states with the nesting vector $\boldsymbol{Q}$ (Q group). The states in this group are expected to always compete with one another irrespective of the detail of models whenever the nesting works relevantly. On the other hand, since the exchange term J favors the FM state, Fig. 1 in [1] is modified as pointed out by KB (see Fig. 1) when the possibility of the FM state is included. We, however, note that this FM instability mainly comes from the peculiarity of our simple model besides the presence of J, i.e., the divergence of the density of states (DOS) at $E = 0$. Actually, no precursor of the FM instability has been observed experimentally in pure URu_2Si_2 [4,5]. In this regard, our model in [1] is too simple to correctly describe this feature in real URu_2Si_2, although it is enough to grasp the essence of the d-SDW. In a more realistic model [6], the FM instability is expected to be less dominant compared with the simple one.



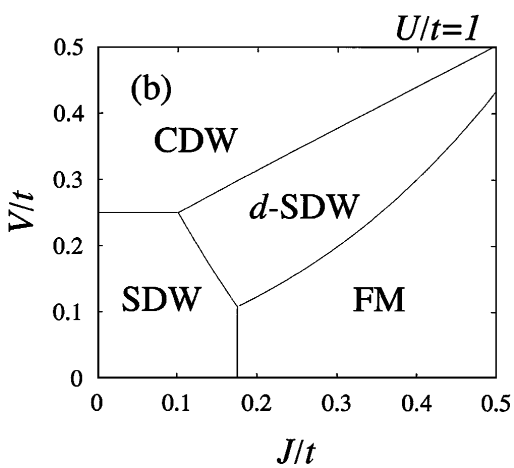


FIG. 1. (a) U-V phase diagram at $J/t = 0.2$. The FM is stable in small U and V. (b) J-V phase diagram at $U/t = 1$.

Next, we discuss the stable region of the d-SDW within Eq. (1) in [1]. As noted in [1], the micromagnetism occurs after the formation of the heavy fermion state. Equation (1) in [1] should be regarded as the effective Hamiltonian for, not the bare electrons, but the quasiparticles with the renormalized interactions, U, V, J. We can expect that U is renormalized to be the order of the quasiparticle bandwidth and $V, J < U$ [5]. Then, there exists a stable d-SDW region as shown in Fig. 1, even if the possibility of the FM state is included.

In conclusion, the possibility of the FM state modifies the phase diagram in [1]. Since this strong FM enhancement is peculiar to our model, further careful analyses may be necessary in constructing more realistic models for URu_2Si_2. However, the physical properties of the d-SDW obtained in [1] themselves are not altered at all by the presence of the FM state, so that the unconventional SDW is still a candidate for the curious magnetism in URu_2Si_2.

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[2] M. N. Kiselev and F. Bouis, preceding Comment, Phys. Rev. Lett. **82**, 5172 (1999).
[3] Since there should exist many Fermi surfaces in URu_2Si_2, the interband nesting is expected in the real system as in the case of Cr. Indeed, in the band calculation, the presence of two electron surfaces around the Γ point and two hole surfaces around the Z point is reported; G. J. Rozing *et al.*, Phys. Rev. B **43**, 9515 (1991). These Fermi surfaces seem to be nested with each other.
[4] M. B. Maple *et al.*, Phys. Rev. Lett. **56**, 185 (1986).
[5] The FM state is observed in the impure system $URu_{2-x}Re_xSi_2$; M. S. Torikachvili *et al.*, Phys. Rev. B **45**, 2262 (1992). This implies that the J term exists to some extent.
[6] For instance, in an extended 2-band Lomar model which is well known as a realistic model for the SDW in Cr [see E. Fawcett, Rev. Mod. Phys. **60**, 209 (1988)], the FM state becomes less important when compared with the case of the single band model because of the absence of singularity in DOS. In this case, the Q group can be favorable unless we choose extremely large J.

