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:

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

where we used the same notations as in [1] except $\vec{S}_i=\frac{1}{2}\sum_j \sigma c_{j\sigma} c_{i\sigma}$. Unlike the conventional SDW, the order parameter $\Psi^Q_0 \equiv \sum_{\sigma} \sigma \langle c_{k+Q\sigma} c_{k\sigma} \rangle$ in the unconventional SDW (d-SDW) [1] state is characterized by "d-wave" like k-dependence $\Psi^Q_0 \propto \cos k_x - \cos k_y$ [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 on 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 $U$-$Pt_3$ and $U$-$Ru_2$Si$_2$ [3]) 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 (*) [4] 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]: $\chi_0(q,0) = \chi_0^D(q,0)/(1 - \chi_0(q)\chi_0^D(q,0))$, where $\alpha=$FM, DW, $I_{FM}(0)=U+4J$, $I_{SDW}(Q)=U-4J$, $I_{CDW}(Q)=8V-U-4J$ and $I_{d-SDW}(Q)=V$. For the perfect nesting case $\chi_0^D(Q,0) \sim (1/t) \log^2(t/T)$ [1], where one power of logarithm comes from nesting and another one is due to the Van Hove singularity (VHS). Nevertheless, $\chi_0^F(0,0) \sim (1/t) \log(t/T)$ is also singular [5] due to VHS. The MF critical temperatures are $T_{DW}^{MF} \sim t$ exp$(-2\pi \lambda_{DW} \sqrt{U/T})$ and $T_{FM}^{MF} \sim t$ exp$(-2\pi \lambda_{FM} t/I_{FM})$, $\lambda_{Q} \sim 1$. Thus, the FM state certainly wins when $J \gg (U,V)$ and $V/J \ll J/t$ 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 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 $t \sim m_s^{-1} < t_0$ ($m_s \gg m_0$ 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 constraint $n_i=1$, nesting is not important and only the AF state with $I_{AF} \sim |t|^2/U$ [6] 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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M.N. Kiselev and F. Bouis
Laboratoire Léon Brillouin, CE-Saclay 91191 Gif-sur-Yvette Cedex, France

[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 no true transition to a state with long range order in a 2D system with a continuous symmetry except for $T=0$.
[4] There is no any unconventional SDW state for $J \leq 0$.
[5] For simplicity we use the random phase approximation.
[6] J.E. Hirsh, Phys. Rev. B 31, 4403 (1985).
[7] 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.
[8] There is no true transition to a state with long range order in a 2D system with a continuous symmetry except for $T=0$.