

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

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We propose a novel spin density wave (SDW) state as a possible mechanism of the anomalous antiferromagnetism, the so called micromagnetism, in URu₂Si₂ below 17.5 K. In this new SDW, the electron-hole pair amplitude changes its sign in the momentum space as in the case of the unconventional superconductivity. It is shown that this state can be realized in an extended Hubbard model within the mean field theory. We also examine some characteristic properties of this SDW to compare with the experimental results. All these properties well explain the unsolved problem of the micromagnetism. [S0031-9007(98)07466-3]

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Electronic states in the U-based heavy fermion compounds UPt₃ and URu₂Si₂ have recently attracted much attentions because of their curious physical properties. The antiferromagnetism is one of them: (1) Magnitude of the induced staggered magnetic moment is extremely small; it is about 0.02μ_B for UPt₃ (T_N = 5 K) [1,2] while 0.04μ_B for URu₂Si₂ (T_N = 17.5 K) [3,4]. They are about 1% of the values expected from the magnetic susceptibility at high temperatures [5,6]. (2) The phase transition can be observed by the neutron scattering [1,3] and the magnetic x-ray diffraction [2,4] in both the materials; in the case of UPt₃, however, it is not detected by other probes, NMR T₁⁻¹ [7], the susceptibility, and the specific heat [5]. On the other hand, a clear jump in the specific heat at T_N and rapid decreases in NMR T₁⁻¹ and in the susceptibility below T_N can be observed in the case of URu₂Si₂. This indicates that, at least for URu₂Si₂, a magnetic phase transition really occurs at T_N.

Although various mechanisms have been proposed in order to explain this *micromagnetism* [8–10], this problem still remains to be settled. Since the antiferromagnetism continues to exist even in the unconventional superconducting phase, this problem is also related to the mechanism of the superconductivity in these materials.

Motivated by this situation, we study the micromagnetism and propose a new mechanism in this paper. We mainly focus on URu₂Si₂, because its phase transition is well confirmed compared with UPt₃ as noted in the above. Namely, we study *how the tiny moment and clear anomalies in some physical quantities can coexist without any inconsistency*.

Unconventional spin-density wave.—First of all, we explain the outline of our idea. (1) In the spin-density wave (SDW), the ordered magnetic moment M_Q is given by

$$M_Q = \sum_k \Psi_k^Q, \quad (1)$$

where $\Psi_k^Q \equiv \sum_{\sigma} \sigma \langle c_{k\sigma}^{\dagger} c_{k+Q\sigma} \rangle$ is the electron-hole pair correlation. (Q represents a characteristic wave vector of the SDW.) In the ordinary simple SDW, Eq. (1) is finite, because Ψ_k^Q is a positive constant and is independent of k. (2) In this paper, we notice the k dependence of Ψ_k^Q , and propose an *unconventional SDW* where Ψ_k^Q changes its sign depending on k; for example, the d-wave symmetry $\Psi_k^Q \propto \cos k_x - \cos k_y$ as in the case of the d-wave superconductivity. In this case, Eq. (1) gives M_Q = 0, because Ψ_k^Q is canceled in the k summation due to its sign change. (3) Presence of Ψ_k^Q decreases the excitation spectrum below the energy gap, even if Ψ_k^Q is anisotropic and M_Q is absent. Then, this energy gap should induce a *large anomaly* in, for example, the specific heat. Thus, “absence of the ordered magnetic moment and presences of large anomalies in some thermodynamic quantities” can be realized in the *unconventional SDW*.

This is our basic idea for the micromagnetism in URu₂Si₂. In the next section, we present a concrete example of this state based on a simple model.

Formulation.—Since the micromagnetism occurs after the heavy fermion was formed [6,11,12], we examine the quasiparticle state described by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle} \sum_{\sigma \sigma'} n_{i\sigma} n_{j\sigma'} + J \sum_{\langle ij \rangle} \sum_{\sigma \sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} c_{i\sigma'} c_{j\sigma}, \quad (2)$$

where $c_{i\sigma}^{\dagger}$ is the creation operator of a quasiparticle and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. The band structure is controlled by the hopping term in Eq. (2), in which $\langle ij \rangle$ represents the summation over nearest-neighbor pairs; although URu₂Si₂ is a three dimensional material and should have a complex band structure, we use a two-dimensional simple square lattice in order to grasp the essence of the unconventional

SDW. Furthermore, we put the chemical potential μ equal to zero: The Fermi surface is then in the perfect nesting with $\mathbf{Q} = (\pi, \pi)$. On the other hand, we take into account three kinds of interactions: the on-site Coulomb repulsion U , the nearest-neighbor direct interaction $V (> 0)$, and the exchange one $J (> 0)$.

Within the mean field theory, the most possible ordered states which may be realized in Eq. (2) are the conventional SDW, the charge-density wave (CDW), and three kinds of novel SDW's, all of that characterized by the nesting vector, $\mathbf{Q} = (\pi, \pi)$ [13]. The mean field Hamiltonian for Eq. (2) is then given by

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{2} \sum_k [\Delta^{\text{CDW}} \rho_{kk+\mathbf{Q}} + \text{H.c.}] + \frac{1}{2} \sum_{k\alpha} [\Delta_{k\alpha}^{\text{SDW}} \sigma_{kk+\mathbf{Q}}^\alpha + \text{H.c.}], \quad (3)$$

where $\xi_k = -2t(\cos k_x + \cos k_y)$, $\rho_{kk+\mathbf{Q}} = c_{k1}^\dagger c_{k+\mathbf{Q}1} + c_{k1}^\dagger c_{k+\mathbf{Q}2}$, and $\sigma_{kk+\mathbf{Q}}^\alpha = c_{k1}^\dagger c_{k+\mathbf{Q}1} - c_{k1}^\dagger c_{k+\mathbf{Q}2}$. (We have chosen the direction of the SDW order parameters being parallel to the z axis without loss of generality.) The CDW order parameter, Δ^{CDW} , and the four SDW ones specified by the channel index α , $\Delta_{k\alpha}^{\text{SDW}}$, are respectively given by

$$\begin{cases} \Delta^{\text{CDW}} = \frac{8V - U - 4J}{2} \sum_{k'\sigma} \langle \rho_{k'+\mathbf{Q}k'} \rangle, \\ \Delta_{k\alpha}^{\text{SDW}} = \frac{I_\alpha}{2} \sigma_k^\alpha \sum_{k'\sigma} \phi_{k'}^\alpha \langle \sigma_{k'+\mathbf{Q}k'}^\alpha \rangle. \end{cases} \quad (4)$$

In Eq. (4), ϕ_k^α and I_α , respectively, represent the basis function which determines the symmetry of the order parameter and the corresponding pairing interaction. For the conventional “ s -wave” SDW, $\phi_k^s = 1$, and $I_s = U - 4J$. On the other hand, the nearest-neighbor direct interaction in Eq. (2) gives three possible “unconventional” SDW's: (1) d wave, $\phi_k^d = \cos k_x - \cos k_y$; (2) extended s wave, $\phi_k^{ex} = \cos k_x + \cos k_y$; (3) p wave, $\phi_k^p = \sqrt{2} \sin k_{x,y}$. All the three states have the same pairing interaction, $I_\alpha = V$.

All the states obey the same form of the self-consistency equation,

$$1 = I_\alpha \sum_k \frac{\phi_k^{\alpha 2}}{2E_k} \text{th} \frac{E_k}{2T} \quad (5)$$

$$(E_k = \sqrt{\xi_k^2 + |\Delta_{k\alpha}^{\text{SDW}}|^2}).$$

(For the CDW, we replace $I_\alpha \rightarrow 8V - U - 4J$ and $\Delta_{k\alpha}^{\text{SDW}} \rightarrow \Delta^{\text{CDW}}$.) Then, neglecting the anisotropy of the Fermi surface and comparing the pairing interactions only, we immediately find that the unconventional SDW's are the most stable in the range of $U - 4J < V < (U + 4J)/7$ [13]. Anisotropy of the Fermi surface widens this region, and furthermore the d wave SDW becomes

the most favorable among the unconventional SDW's, because the d -wave basis function, $\phi_k^d = \cos k_x - \cos k_y$, has a large value at the corner of the Fermi surface at which the density of states diverges. We demonstrate a typical U - V phase diagram at $J = t$ in Fig. 1. Clearly, there exists a stable region of the d -wave SDW which is wider than that of the above simple evaluation.

At this stage, it is difficult to evaluate U , V , and J for URu_2Si_2 . However, in real materials, at least the on-site U should be larger than the other nearest-neighbor interactions, V and J . Figure 1 shows that the d -wave SDW can be realized even under this physical restriction, $U > V, J$. Thus, the d -wave SDW can be considered as a possible state in real systems.

Physical properties of the d -wave SDW.—Let us proceed to the detail analysis of some physical properties of the d -wave SDW comparing with the conventional s -wave one. In what follows, we simply write $\Delta_{k\alpha=d,s}^{\text{SDW}}$ as $\Delta_k^{d,s}$.

(1) *SDW order parameter.*—The d -wave SDW order parameter, Δ_k^d must be a purely imaginary number contrary to the conventional SDW, because Δ_k^d satisfies $(\Delta_k^d)^* = -\Delta_k^d$ due to $\phi_{k+\mathbf{Q}}^d = -\phi_k^d$. (Note that one cannot choose the phase of the order parameter freely in contrast to the case of the superconductivity.) Because of this property, the d -wave SDW has a finite spin current as pointed out by Ozaki [13].

Figure 2 shows the temperature dependence of the SDW order parameter. It is found that there is no essential difference in between the d -wave SDW and the s -wave one. In the d -wave case, the ratio of the order parameter to T_N is

$$\frac{2\Delta_{\text{max}}}{T_N} \approx 4.8 \quad [\Delta_{\text{max}} \equiv \max(|\Delta_k^d|)]. \quad (6)$$

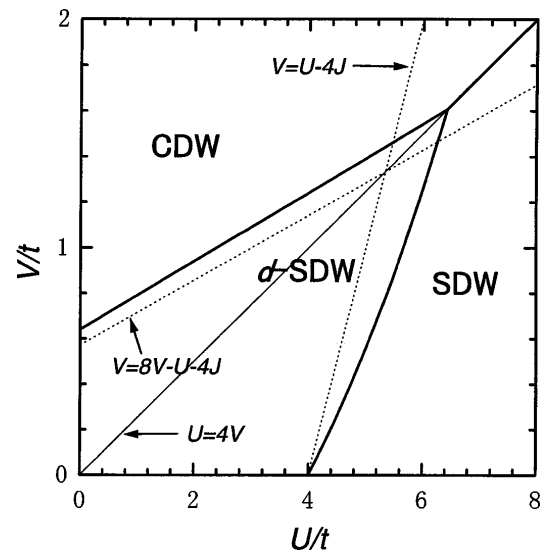


FIG. 1. U - V phase diagram at $J = t$. All the states in the figure are characterized by the nesting vector $\mathbf{Q} = (\pi, \pi)$.

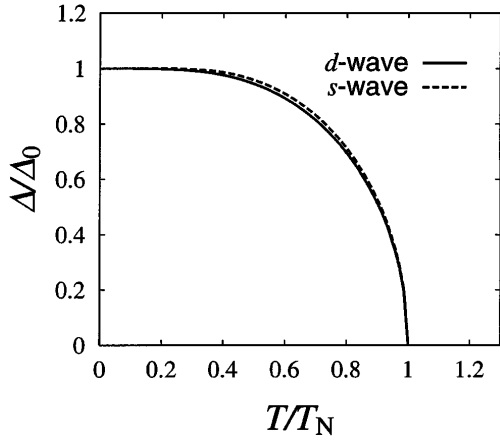


FIG. 2. Temperature dependence of the order parameter normalized by $\Delta_0 \equiv \Delta(T=0)$ of each state. Relation between Δ in the figure and the order parameter is $\Delta_k^d = i\phi_k\Delta$ in the case of the d wave. We put $(U-4J)/t = V/t = 2$, which gives $T_N \approx 0.4t$ ($0.2t$) for the d wave (s wave). We also use the same parameter set in Fig. 3.

Thus this state has a large excitation gap with the order of T_N . Such a gap is actually observed by the inelastic neutron scattering [3,4]. (Strictly speaking, since the d -wave order parameter has nodes, the density of states is not completely absent even below Δ_{\max} .)

(2) *Thermodynamic properties.*— We examine how the presence of the excitation gap affects the thermodynamic property below T_N . Here, we show two examples: (A) Figure 3(a): specific heat C .

$$C(T) = \sum_k \left(\frac{E_k^2}{T} - \frac{1}{2} \frac{d|\Delta_k^{d,s}|^2}{dT} \right) \frac{d}{dE_k} \text{th} \frac{E_k}{2T}. \quad (7)$$

The specific heat shows a discontinuous jump at T_N as in the case of the conventional SDW. The origin of the jump is the $d|\Delta_k^{d,s}|^2/dT$ term in Eq. (7) because of $|\Delta_k^{d,s}| \propto \sqrt{T_N - T}$ near T_N .

(B) Figure 3(b): uniform susceptibility χ_0 .

$$\begin{cases} \chi_{0\parallel} = \frac{1}{2} \sum_k \frac{d}{dE_k} \text{th} \frac{E_k}{2T}, \\ \chi_{0\perp} = \frac{1}{2} \sum_k \left(\frac{|\Delta_k^{d,s}|^2}{E_k^3} \text{th} \frac{E_k}{2T} + \frac{\xi_k^2}{E_k^2} \frac{d}{dE_k} \text{th} \frac{E_k}{2T} \right), \end{cases} \quad (8)$$

where $\chi_{0\parallel}$ ($\chi_{0\perp}$) is the parallel (perpendicular) component to the z axis. $\chi_{0\perp}$ is almost constant below T_N , while $\chi_{0\parallel}$ shows a rapid decrease due to the reduction of the density of states below the energy gap; their behaviors are just equal to those in the usual antiferromagnetism.

Since the density of states behaves like $N(E) \propto E(E \sim 0)$ in the case of the d -wave SDW, C and χ_0 show power-law temperature dependences at $T \ll T_N$ as $C \propto T^2$ and $\chi_{0\parallel} \propto T$. On the other hand, they show exponential decreases in the case of the conventional s -wave SDW due to the finite excitation gap.

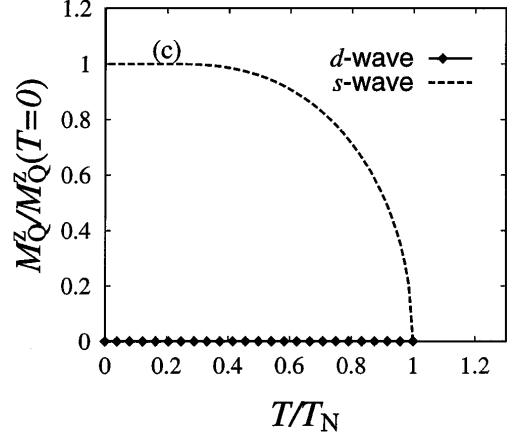
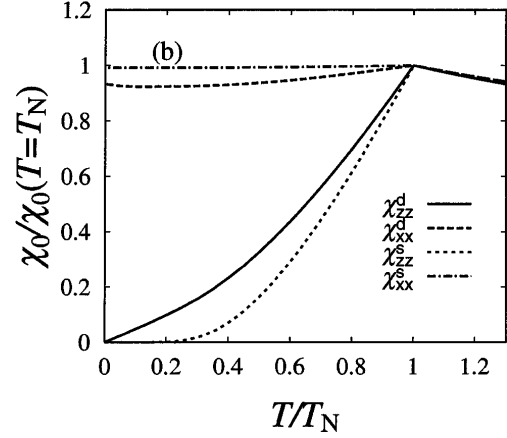
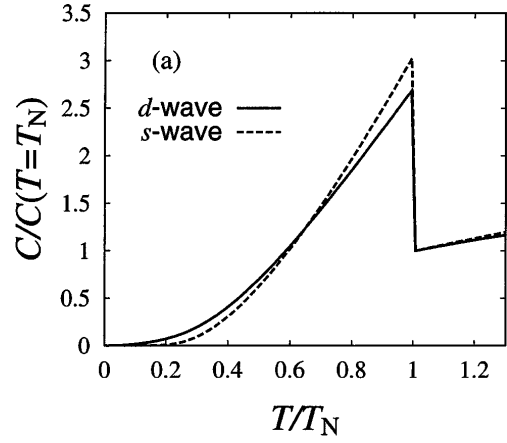


FIG. 3. Temperature dependences of (a) the specific heat, (b) the uniform susceptibility, and (c) the staggered magnetic moment. These are, respectively, scaled to $C(T=T_N+0)$, $\chi_0(T=T_N)$, and $M_Q^z(T=0)$. In each figure, the temperature is normalized by T_N of each state; the discrepancy in $T > T_N$ arises from the difference of T_N in between the s wave and the d wave. In (b), χ_{zz} and χ_{xx} are, respectively, $\chi_{0\parallel}$ and $\chi_{0\perp}$ in this text.

(3) *Magnetic moment.*— The staggered magnetic moment is given by

$$M_Q^z = \sum_k \langle \sigma_{kk+Q}^z \rangle = \sum_k \frac{\Delta_k^{d,s}}{2E_k} \text{th} \frac{E_k}{2T}. \quad (9)$$

In the case of d -wave SDW, Eq. (9) always vanishes because of $\Delta_k^d \propto \phi_k^d$. Namely, the spin density itself is homogeneous in spite of the name “spin density wave” [14]. We emphasize that the absence of M_Q^z is qualitatively different from the case of the conventional s -wave SDW in which M_Q^z is essentially equivalent to the order parameter. We show their qualitative difference in Fig. 3(c).

The absence of M_Q^z means that the antiferromagnetic susceptibility does not diverge at T in contrast to the conventional s -wave SDW. In the latter case, the divergence leads to a deviation of NMR T_1^{-1} from the Korringa-like temperature dependence. On the other hand, the $T_1^{-1} \propto T$ is expected up to just above T in the d -wave SDW because of the absence of the divergence in the spin susceptibility. This result agrees with the experiment [7].

How does the “micro-” but “finite-” staggered moment appear in the present d -wave SDW? We have two answers for this question: (1) When the lattice is deformed to some extent, the cancellation of the summation in Eq. (9) becomes incomplete because of the deformation of the Fermi surface. Then M_Q^z can be finite. In this case, the staggered magnetic moment may strongly depend on the applied pressure; such a behavior is actually reported in UPt_3 [15]. (2) Since the unconventional SDW should be destroyed near impurities and boundaries, the s -wave SDW may be induced around them by the proximity effect, as in the case of the superconductivity. In this case, we obtain a finite staggered magnetic moment with a short range correlation, because the staggered magnetic moment which accompanies the s -wave component localizes around the defects. We explain details of these mechanisms in our forthcoming paper [16].

In summary, we have proposed a novel SDW characterized by the electron-hole pair amplitude changing its sign in the momentum space as a possible mechanism of the micromagnetism in URu_2Si_2 . This kind of unconventional SDW shows clear anomalies in the specific heat and the uniform susceptibility as in the case of the usual SDW, while the induced staggered magnetic moment is absent. We emphasize that these results well explain the properties of the micromagnetism in URu_2Si_2 . Although we examined the d -wave SDW in two dimension as a simple example, the essential results in this paper describe general property of the unconventional SDW.

Finally, we briefly comment on UPt_3 which has no anomaly in, for instance, the specific heat. When we consider the order parameter which is zero at the Fermi surface, such as an extended s -wave symmetry or an odd- ω state discussed in the field of superconductivity, the jump in the specific heat becomes small or absent. Thus, we can expect that the unconventional SDW is a possible mechanism also for the micromagnetism in this material.

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