Interplay between SDW and induced local moments in URu$_2$Si$_2$

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Theoretical model for magnetic ordering in the heavy-fermion metal URu$_2$Si$_2$ is suggested. The 17.5 K transition in this material is ascribed to formation of a spin-density wave, which develops due to a partial nesting between electron and hole parts of the Fermi surface and has a negligibly small form-factor. Staggered field in the SDW state induces tiny antiferromagnetic order in the subsystem of localized singlet-singlet levels. Unlike the other models our scenario is based on coexistence of two orderings with the same antiferromagnetic dipole symmetry. The topology of the pressure phase diagram for such a two order parameter model is studied in the framework of the Landau theory. The field dependences of the staggered magnetization and the magnon gap are derived from the microscopic theory and found to be in good quantitative agreement with experiment.

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I. INTRODUCTION

URu$_2$Si$_2$ is one of the most intriguing heavy-fermion compounds. It exhibits a sharp second-order transition at $T_m = 17.5$ K, which has pronounced effect on thermodynamic and kinetic properties. Though the neutron diffraction experiments$^{6,7,8,9}$ and the X-ray magnetic scattering measurements$^{10}$ have produced evidence for only tiny staggered moments $\mu \simeq 0.02-0.04 \mu_B$ at $Q = (1,0,0)$. Magnetic excitations observed by inelastic neutron scattering experiments$^{6,8}$ are reasonably well explained within the model with exchange interaction in a singlet-singlet Van-Vleck paramagnet. This model fails, however, to give a consistent description of the ordering temperature and small ordered moments unless the exchange interaction $J_Q$ is accidentally close to a critical value (see section IV below). A weak antiferromagnetic ordering of a Van Vleck paramagnet cannot produce a measured jump in the specific heat and an electrical resistivity anomaly. These experimental features rather resemble formation of a spin-density wave (SDW), which involves approximately a half of the Fermi surface. In its turn, the SDW scenario is inconsistent with a longitudinal polarization of the magnetic excitations. As a result of this contradiction, various theoretical scenarios have been proposed in the past to explain intriguing behavior of URu$_2$Si$_2$.$^{11,12,13,14,15,16,17,18,19,20,21,22,23,24,25}$

The proposed theories of URu$_2$Si$_2$ can be crudely divided into three broad categories. Phenomenological models of the first group$^{15,20}$ take pragmatic approach and introduce a yet unknown primary or hidden order parameter $\psi$, which drives the 17.5 K transition and is responsible for a large specific heat anomaly at $T_m$. Small ordered moments observed in the neutron experiments are described by a secondary Ising-like antiferromagnetic order parameter $m$. Depending on the symmetry of the hidden order parameter different coupling terms of the type $\psi m$ and $\psi^2 m^2$ are possible in the Landau energy functional. In particular, the model with a bilinear term predicts a nontrivial field-dependence of weak antiferromagnetic moments with an inflection point. Subsequent neutron measurements have nicely confirmed such a prediction.$^{24}$

Second group of theories consists of specific proposals for the hidden order parameter. These models are further subdivided into two subgroups. The first subgroup includes models, in which the primary order parameter breaks the time-reversal symmetry. These are spin-density waves in higher angular momentum channels$^{13,19}$ and ordering of octupolar moments on uranium sites.$^{22}$ For such theories the bilinear coupling term with the antiferromagnetic vector is, in principle, possible, though some other crystal symmetries are required to be absent. The second subgroup includes theoretical models with a time-reversal invariant hidden order parameter such as quadrupolar$^{16}$ or spin nematic ordering.$^{14}$ In such a case the bilinear term is prohibited by symmetry and only a biquadratic interaction exists between the two order parameters.

The last third group of theoretical works includes attempts to realistically describe the microscopic interactions in URu$_2$Si$_2$. A so called Ising-Kondo lattice model$^{25}$ describes interaction between conduction electrons in nested bands and local crystal-field split moments. The mean-field calculation produces both a weak moment and an appropriate value of the transition temperature but does not reproduce the large specific heat jump. A closely related dual model$^{25}$ considers a subsystem of localized singlet-singlet levels and a subsystem of itinerant electrons with a similar assumption on the nesting condition. A better description of the thermodynamic properties of URu$_2$Si$_2$ has been achieved by adding the superexchange and the RKKY interactions between local moments. The field behavior still remains largely inconsistent with the experimental measurements.$^{24,25}$

Further development of the dual model has been recently suggested in Ref. 25. Note, that the above two microscopic models (i) completely neglect the Coulomb interaction between charge carriers and (ii) operate with a single (antiferromagnetic) order parameter.

Up to now experiments have been unable to distin-
guish between the competing theoretical proposals. Two potentially important experimental developments published recently include pressure experiments and the NMR measurements. Investigations under hydrostatic pressures have shown that the $P-T$ phase diagram is divided into two regions: a small moment antiferromagnetic phase (SMAF) at low pressures and a large moment antiferromagnetic phase (LMAF) at high pressures with a first-order transition line in between. Such a discovery is generally consistent with phenomenological two order parameter scenarios for URu$_2$Si$_2$ (see section III, below). Another experimental finding came out from the NMR measurements. Matsuda and co-workers have found that a paramagnetic Si NMR absorption line persists well below $T_m$ accompanied by two much smaller peaks symmetrically shifted by antiferromagnetic field. Such an observation points at an inhomogeneous para-antiferromagnetic state below the 17.5 K transition. The peak intensities suggest that about 97% of the sample volume is in a paramagnetic state. The puzzle of small uranium moments in URu$_2$Si$_2$ seems to be reinterpreted as due to a phase separation between nonmagnetic state with a hidden order and small antiferromagnetic droplets with ordinary (large) value of staggered magnetization. Such a simple explanation of the main mystery of URu$_2$Si$_2$ is quite appealing but leaves without answer question why the inhomogeneous phase exists not only in the vicinity of the first-order transition line at high pressures, but in the whole region of SMAF. The development of the antiferromagnetic Bragg peaks right below $T_m = 17.5$ K seems to be highly accidental in the phase separation scenario. Also, an inflection point in the field dependence of antiferromagnetic Bragg peaks cannot be explained if small peaks are purely due to a volume effect. Thus, physical implications of the NMR measurements are not completely straightforward and have to be further clarified.

In this paper, we present a semimicroscopic model for URu$_2$Si$_2$, which is closely related to the above mentioned dual models but operates with two order parameters in the spirit of phenomenological scenarios. We also consider two magnetic subsystems: (i) local crystal-field split moments on U$^{4+}$ sites and (ii) conduction electrons in nested bands. In contrast to the previous works, we assume that the electron-electron interaction is non-negligible and that it drives a SDW transition in the nested parts of the Fermi surface. The critical temperature $T_m = 17.5$ K is associated with $T_{SDW}$ and the SDW amplitude $\psi$ plays the role of a primary (hidden) order parameter. According to the LSDA calculations, the nesting wave-vector is commensurate and corresponds to the experimentally observed two-sublattice antiferromagnetic structure. The SDW formed in conduction bands is responsible for large changes in thermodynamic and kinetic properties of URu$_2$Si$_2$. At the same time, we argue that the SDW has a small form-factor and does not create significant Bragg reflection. Local polarization of uranium sites by a staggered magnetic field from the SDW induces tiny antiferromagnetic moments. The magnetic dynamics probed by neutrons is also determined by a localized subsystem.

By making a single assumption about a hidden order parameter with the same symmetry as the observed antiferromagnetic ordering, we have further derived several results, which allow detailed comparison with available measurements and suggest future experimental tests:

(i) The $P-T$ phase diagram with line of the first order type transition, which terminates at the critical point below $T_m(P)$;

(ii) Field dependence of staggered magnetization coincides perfectly with the experimental data for a realistic set of microscopic parameters;

(iii) Field dependence of the excitation spectrum.

The article is organized as follows. In section II, we introduce the model and discuss various features of the spin-density wave instability specific for URu$_2$Si$_2$. In section III, using the phenomenological approach with an appropriate Landau energy functional for two coexistent order parameters we investigate the topology of the $P-T$ phase diagram of URu$_2$Si$_2$. In the next section, a system of localized crystal-field split singlet-singlet levels is considered under combined influence of a uniform external magnetic field and a staggered “internal” field induced by the SDW. We calculate the field dependences of the staggered magnetization and the excitation spectrum. Comparison to the experimental data is presented in section V, which is followed by discussion and conclusions.

II. SPIN-DENSITY WAVE

An unusual assumption made by phenomenological theories is a description of URu$_2$Si$_2$ with two order parameters having the same symmetry. On the first site such an assumption contradicts to a general spirit of the Landau theory of phase transition. Recent investigations of a two-gap superconductor MgB$_2$ have, however, demonstrated usefulness of the description of the superconducting state by means of two weakly interacting s-wave condensates of the Cooper pairs (see, for instance, Ref. 51). The necessary condition for this is a significant mismatch of the pairing interactions in the two bands. In the absence of interband scattering of the Cooper pairs, each band has its own superconducting transition temperature. An interband interaction is always present in real metals and leads to a single transition into a state with two different gaps. The two gaps (order parameters) still keep different dependences on temperature, pressure and/or applied magnetic field. In relation to URu$_2$Si$_2$, the two order parameters $\psi$ and $m$ should correspond to two significantly different magnetic subsystems. We suggest here that the primary order parameter may be an ordinary SDW. The common objections against a SDW transition are (i) smallness of ordered moments and (ii) longitudinal polarization of sharp magnetic excitations. This two properties can be reconciled with a SDW sce-
nario by taking into account specific features of URu$_2$Si$_2$. In this section we discuss the former feature, while the properties of magnetic excitations are considered in section IV.

The early experimental works on the specific heat and the magnetoresistance in URu$_2$Si$_2$ have found strong evidences in favor of a charge or a spin-density wave instabilities in the heavy-electron subsystem at $T_m = 17.5$ K. The fit of the electronic specific heat below the transition indicates that a gap $\Delta_0 \simeq 130$ K develops on 40% of the Fermi surface at $T \to 0$. This conclusion has received a strong support from the de Haas van Alphen (dHvA) measurements. Comparison of the measured dHvA frequencies to the ab-initio band structure shows that two large pieces of the Fermi surfaces, band-18 hole and band-19 electron, are not observed at low temperatures, probably due to their partial removal below the ordering temperature. The above two sheets have nearly spherical shapes and are separated by a nesting wave-vector $Q = (0, 0, 1)$, which is equivalent to $(1, 0, 0)$ in the Brillouin zone of a body-centered tetragonal lattice. Direct calculation of a static momentum-dependent susceptibility also shows a peak at the commensurate wave-vector $Q = (1, 0, 0)$.

A fast decrease of the uniform susceptibility below $T_m$ as well as suppression of the transition temperature $T_m$ and the bulk gap $\Delta_0$ by applied magnetic field also point to a charge- or a spin-density wave state. For the CDW the Zeeman splitting degrades the nesting of the Fermi surfaces and reduces a mean-field transition temperature in a way, which is analogous to the paramagnetic limit effect in superconductors. By contrast, an isotropic SDW involves coupling of bands with opposite spin and the nesting is not affected by a magnetic field. A strong spin-orbit coupling in heavy-fermion materials creates momentum dependence of the $g$-factor. If the nesting condition $\epsilon(k + Q) = -\epsilon(k)$ is satisfied for particular sheets of the Fermi surface it is not generally fulfilled for the Zeeman shift $\mu_B g_S(k + Q)/\hbar \neq \mu_B g_S(k)/\hbar$. Hence, in metals with strong spin-orbit coupling an SDW state is also suppressed by the paramagnetic effect.

The mean-field theory of a SDW formation in Ideally magnetic limit effect in superconductors. By contrast, an $s$-wave superconductor. Their results indicate that in a wide range of impurity concentration, the jump in the specific heat and the transition temperature are suppressed at approximately the same rate, hence, preserving the BCS estimate for the relative specific heat jump. Second, the electron mass enhancement in heavy fermion materials ($m^*/m \sim 25$ in URu$_2$Si$_2$) can significantly reduce the Fermi energy scale $\varepsilon_F$. However, simultaneously with a mass renormalization, an interaction with spin fluctuations reduces strongly the spectral weight of heavy quasiparticles adding an extra small factor $(m/m^*)^3$ to Eq. (1), which completely compensates the factor $(m^*/m)$ in the density of states and further reduces value of the ordered moments. Finally, according to the band structure calculations URu$_2$Si$_2$ is a compensated metal with equal number of electrons and holes. The number of carriers in the two bands undergoing a SDW transition is smaller than one, when normalized to the number of U-atoms. This yields an extra reduction factor, since the neutron scattering experiments report the ordered moments normalized per one uranium.

The above arguments can, in our view, convincingly explain why small antiferromagnetic Bragg peaks in URu$_2$Si$_2$ are consistent with a SDW instability. In the following we assume that due to nesting between some parts of the Fermi surface in URu$_2$Si$_2$ the commensurate SDW state is formed below the critical temperature $T_m$ and that the SDW amplitude $\psi \sim \sum_k \langle \sigma^z_k \rangle / (\varepsilon_k + Q \varepsilon_k)$ plays the role of a hidden order parameter in the problem.

### III. Phase Diagram Under Pressure

The microscopic dual model assumes that conduction electrons are noninteracting and operate, therefore, with a single order parameter, which leaves no place for the phase diagram with SMAF and LMAF regions. In...
our scenario, temperatures of intrinsic phase transitions in itinerant and localized magnetic subsystems are different functions of $P$ and they may interchange their order under pressure. As a result, a line of first-order transitions appears naturally between the two ordered states, where one order parameter prevails over another, see Fig. 4.

The Landau free-energy for two interacting order parameters can be written as

$$F = \alpha_1 \psi^2 + \alpha_2 m^2 + 2 \gamma \psi m + \beta_1 \psi^4 + \beta_2 m^4 + 2 \beta_3 \psi^2 m^2. \quad (2)$$

A special bilinear coupling term is allowed only if the two parameters transform according to the same irreducible representation, otherwise $\gamma \equiv 0$. For nonzero $\gamma$, the quantities $\psi$ and $m$ do not correspond to two different types of symmetry breaking. Rather they describe two weakly coupled magnetic subsystems of URu$_2$Si$_2$ in a way, which is reminiscent of the Ginzburg-Landau description of the multigap superconductivity in MgB$_2$. The bilinear term corresponds, then, to a polarization of local moments by a spin-density wave.

Generally, in addition to the bilinear term $\psi m$ there are possible other coupling terms in the Landau functional: $\psi^3 m$ and $\psi m^3$. These terms can exist even if $\psi$ and $m$ transform according to different irreducible representations (though $\psi$ has to break the time-reversal symmetry). The $\psi^3 m$ term leads, for example, to a small antiferromagnetic component in a state with $\psi \neq 0$, even if $\gamma \equiv 0$. The induced $m$ component grows in such a case as $m \sim (T_m - T)^{1/2}$, while the neutron diffraction experiments find a standard mean-field exponent $1/2$ in a way, which is reminiscent of the Ginzburg-Landau description of the multigap superconductivity in MgB$_2$. The bilinear term corresponds, then, to a polarization of local moments by a spin-density wave.

In order to investigate the possible ordered states and phase transitions below $T_m(P)$, one has to minimize Eq. (2) with respect to both $\psi$ and $m$. This gives a system of two coupled cubic equations, which is easily solved numerically, but does not allow full analytic solution. Still, simple analytic arguments can be used to prove stability of the first-order transition line for $\gamma \neq 0$ and $\beta_i > \sqrt{\beta_1 \beta_2}$. [For $\beta_i < \sqrt{\beta_1 \beta_2}$, the bilinear term stabilizes the mixed phase ($\psi \neq 0$ and $m \neq 0$) right below $T_m(P)$.]

Substitution $m \to (\beta_1/\beta_2)^{1/4} m$ transforms the free-energy to a more symmetric form:

$$F = \alpha_1 \psi^2 + \tilde{\alpha}_2 m^2 + 2 \tilde{\gamma} \psi m + \beta_1 (\psi^2 + m^2)^2 + 2 \tilde{\beta}_3 \psi^2 m^2, \quad (4)$$

where $\tilde{\alpha}_2 = (\beta_1/\beta_2)^{1/2} \alpha_2$, $\tilde{\gamma} = (\beta_1/\beta_2)^{1/4} \gamma$, and $\tilde{\beta}_3 = (\beta_1/\beta_2)^{1/2} \beta_3 - \beta_1$. In the new notations the condition for the absence of the mixed phase at $\gamma = 0$ is $\tilde{\beta}_3 > 0$, while the position of the first-order transitions line in the $P-T$ plane is given by $\alpha_1 = \tilde{\alpha}_2$. Let us cross from the paramagnetic state into the ordered state along this line taking $\alpha_1 = \tilde{\alpha}_2 = \alpha$. The transformation $\psi = \eta_1 - \eta_2$,

![Fig. 1: The phase diagram of the two-order parameter Landau functional for $\gamma = 0$ (left panel) and for $\gamma \neq 0$ (right panel).](image)
The relative phase between \( \eta_1 \) and \( \eta_2 \) is not fixed, though solutions \((|\eta_1|, |\eta_2|)\) and \((|\eta_1|, -|\eta_2|)\) describe two essentially different states. Away from the line \( \alpha_1 = \hat{\alpha}_2 \), the energy \((\ref{eq:1})\) acquires the extra term \(2(\alpha_1 - \hat{\alpha}_2)\eta_1\eta_2\), which immediately lifts the above two-fold degeneracy and selects either 0 or \(\pi\) shift between \(\eta_1\) and \(\eta_2\) on the two sides of \(\alpha_1 = \hat{\alpha}_2\). Consequently, the first order transition line \(T_M(P)\) is stable and its position in the \(P-T\) plane is given by the same equation as for \(\gamma = 0\). However, \(T_M(P)\) splits from the line of second order phase transitions \(T_m(P)\) and terminates at the critical point determined by Eq. \((\ref{eq:1})\); see the right panel of Fig. \((\ref{fig:1})\).

The two states to the left and to the right from \(T_M(P)\) are phases with large \(\psi_L = |\eta_1| + |\eta_2|\) and small \(m_S = |\eta_1| - |\eta_2|\) (SMAF) and with small \(\psi_S = |\eta_1| - |\eta_2|\) and large \(m_L = |\eta_1| + |\eta_2|\) (LMAF). A relative jump of the ordered antiferromagnetic moments across \(T_M(P)\) is given by

\[
\frac{m_L - m_S}{m_L + m_S} = \frac{\eta_2}{|\eta_1|} = \frac{\sqrt{\alpha - \alpha(T_m)}}{\alpha + \alpha(T_m)}.
\]

The size of the jump varies continuously along \(T_M(P)\) and vanishes at \(P = P_c\). Note, that the distance between the critical line \(T_m(P)\) and the critical point \(T_c\) given by Eq. \((\ref{eq:1})\) is proportional to \(\gamma\) and may be quite small. At present, the neutron experiments under hydrostatic pressure has failed to identify the critical end point \((T_c, P_c)\) on the line of first-order transitions \(T_M(P)\). We suggest that specific heat measurements can help to finally resolve the phase diagram of URu$_2$Si$_2$.
with $H = H_s = 0$. At zero temperature and in the large gap limit the system remains in a singlet ground state. The excitation spectrum consists of magnetic or Van-Vleck excitons, which are bound states of the two singlet levels. Energy of Van-Vleck excitons is easily found by applying the Holstein-Primakoff representation to pseudo-spin-1/2 operators. In the harmonic approximation it is suffice to write

$$S_i^z = \frac{1}{2} - a_i^\dagger a_i , \quad S_i^x = \frac{1}{2} (a_i^\dagger + a_i) .$$

Eq. (10). At zero temperature the sublattice magnetization is

$$M_{s0} = 2\mu m_{s0} = \mu \sqrt{1 - \frac{\Delta^2}{\Delta_c^2}} ,$$

whereas near $T_N$ the antiferromagnetic moments follow the mean-field temperature dependence:

$$M_s^2 \approx M_{s0}^2 \frac{\Delta^2}{T_N \Delta_c} - \frac{\Delta^2}{2 \Delta_c^2} + \frac{T_N - T}{T_N} .$$

The above equation shows that upon approaching the Ising limit $\Delta \ll \Delta_c$, the dispersion of the longitudinal excitations is gradually diminished. For more details and discussion see the end of the subsection C.

Neutron scattering measurements on URu$_2$Si$_2$ yield a moderate value of the matrix element of the total angular momentum $\mu \approx 1.2 \mu_B$. A simple explanation of small static moments would be, then, to assume that $(\Delta_c - \Delta) \ll \Delta$. According to Eq. (10), such an assumption also leads to a small transition temperature compared to the crystal-field level splitting $T_N \ll \Delta$, which is again in agreement with the experimental observation of $\Delta \approx 10$ meV. The above straightforward explanation of small ordered moments fails, however, to explain a large jump of the specific heat at $T_N$. Indeed, in the molecular-field approximation the specific heat jump at the transition temperature (13) is

$$\frac{\Delta C}{C} = 2T_N \frac{\Delta^2}{\Delta_c} \left| \frac{dm_{s0}}{dT} \right|_{T_N} .$$

Using Eq. (21) we find in the limit $\Delta \to \Delta_c$:

$$\frac{\Delta C}{C} \approx \frac{\Delta_c^2 - \Delta^2}{2 \Delta_c} \ln \frac{\Delta_c + \Delta}{\Delta_c - \Delta} .$$

Taking $M_{s0} \approx 0.03 \mu_B$, which implies that $(\Delta_c - \Delta)/\Delta_c \approx 3 \times 10^{-4}$, we find for the specific heat jump $\Delta C/C \approx 2.7 \times 10^{-3}$. Such a jump is three orders of magnitude smaller than the experimentally measured jump at the 17.5 K transition. Corrections to the molecular-field approximation (24,25) do not significantly modify the jump $\Delta C$. Consequently, it has been concluded that spontaneous ordering of local moments on uranium sites cannot explain the phenomenology of the antiferromagnetic transition in URu$_2$Si$_2$. In the next sections we shall consider the model (13) in the regime of induced local moments, that is $\Delta > \Delta_c = 2\mu^2 |\mathcal{J}_Q|$ and $H_s \neq 0$. 

The wave-vector $Q$ corresponds to the absolute minimum of $\mathcal{J}_k$. Let us emphasize here that neither $\Delta$ nor $\Delta_g$ have any relation to the bulk gap $\Delta_0$, which corresponds to itinerant magnetic subsystem. Quantum fluctuations somewhat renormalize the spectrum (15) at $T = 0$ and tend to further reduce the critical gap $\Delta_c$. This effect depends, however, on a particular form of $\mathcal{J}_k$, and for a three-dimensional system does not exceed 2–3%. Below, we neglect such quantum corrections.

If the crystal field splitting $\Delta$ becomes smaller than $\Delta_c$, the system develops a long-range magnetic order with a staggered magnetization $\langle J^z \rangle = 2\mu (S_i^z) \sim e^{i\mathcal{Q}r_i}$. In the following we always assume that magnetic ordering has a two-sublattice antiferromagnetic structure, that is $e^{2i\mathcal{Q}r_i} = 1$ or $2\mathcal{Q} \equiv 0$ as in URu$_2$Si$_2$. In order to describe a finite-temperature transition in ordered state one can use a simple molecular-field approximation (24,25). For this we write

$$\langle S_i^z \rangle = m_s e^{i\mathcal{Q}r_i} ,$$

where the dimensionless staggered magnetization $m_s$ is determined by a self-consistency equation obtained from a single-site solution:

$$m_s = \frac{2\mu^2 |\mathcal{J}_Q|m_{s0}}{\sqrt{\Delta^2 + 16\mu^4 |\mathcal{J}_Q|^2 m_{s0}^2}} \tanh \frac{\sqrt{\Delta^2 + 16\mu^4 |\mathcal{J}_Q|^2 m_{s0}^2}}{2T} .$$

The transition temperature obtained from the above equation is

$$\frac{\Delta}{T_N} = \ln \frac{\Delta_c + \Delta}{\Delta_c - \Delta} .$$

In the molecular-field approximation the transition temperature vanishes as $\Delta \to \Delta_c - 0$ in agreement with
B. Finite Fields: Mean-field approximation

The mean-field ansatz for a sublattice magnetization in the presence of both uniform $H$ and staggered $H_s$ magnetic fields is given by

$$\langle S_i^z \rangle = m_s e^{i Q r_i} + m_0.$$  \hfill (25)

For a single spin, the mean-field Hamiltonian takes the following form

$$\hat{H}_{MF} = -\Delta S_i^z - S_i^z \left[ (2 \mu H_s + 4 \mu^2 |\mathcal{J}_Q| m_s) e^{i Q r_i} + 2 \mu H - 4 \mu^2 \mathcal{J}_0 m_0 \right],$$ \hfill (26)

where $\mathcal{J}_0 = \mathcal{J}_{k=0}$. Calculating an equilibrium magnetization we find for two sublattices:

$$m_s \pm m_0 = \frac{D_\pm}{\sqrt{\Delta^2 + 4 D_\pm^2}} \tanh \frac{\Delta^2 + 4 D_\pm^2}{2 T},$$

$$D_\pm = \mu (H_s \pm H) + 2 \mu^2 (|\mathcal{J}_Q|m_s \mp \mathcal{J}_0 m_0).$$ \hfill (27)

Below, we focus on the case $\Delta > \Delta_c = 2 \mu^2 |\mathcal{J}_Q|$, where there is no magnetic ordering in the subsystem of local moments down to $T = 0$ in the absence of both external and internal fields. For weak staggered field, linearization of Eq. (27) in $H_s$ and $m_s$ at $H = 0$ yields

$$m_s = \frac{\mu H_s \tanh(\Delta/2 T)}{\Delta - \Delta_c \tanh(\Delta/2 T)}.$$ \hfill (28)

In accordance with the phenomenological formula 3 of section II, weak local moments are proportional to the primary (SDW) order parameter. At zero temperature the dimensional staggered moments are

$$M_{s0} = \frac{2 \mu \mu H_s}{\Delta - \Delta_c}.$$ \hfill (29)

The above equation allows to estimate the staggered field in URu$_2$Si$_2$ from the available experimental data, see section V.

The effect of a uniform field on induced local moments is considered, for simplicity, for $T = 0$ only. In this case expansion of Eq. (27) to linear order in $m_s$ and $H_s$ yields

$$m_s = \frac{\mu H_s}{\Delta(1 + 4 \mu^2 H^2/\Delta^2)^{3/2} - \Delta_c},$$ \hfill (30)

where an effective field $\bar{H} = H - 2 \mu \mathcal{J}_0 m_0$ is determined self-consistently from

$$\bar{H} = H - \frac{2 \mu^2 \mathcal{J}_0 \bar{H}}{(\Delta^2 + 4 \mu^2 H^2)^{1/2}}.$$ \hfill (31)

According to arguments of section III, the SDW contribution to the magnetic Bragg peaks is negligible due to a small form-factor. Then, the measured intensity of Bragg reflections is proportional to $m_s^2$. Suppression of an SDW order parameter with an external field can be described by a simple formula $\psi^2 \propto (1 - H^2/H_s^2)$ or $H_s^2 = H_s^2(1 - H^2/H_s^2)$, where $H_s \approx 40$ T is a metamagnetic field in URu$_2$Si$_2$. The magnetic Bragg peak intensity is

$$I_Q \sim m_s^2 = \frac{\mu^2 H^2}{\sqrt{\Delta(1 + 4 \mu^2 H^2/\Delta^2)^{3/2} - \Delta_c^2}}.$$ \hfill (32)

This zero-temperature result should be compared to the analogous formulas valid near $T_m$, which have been derived in the previous works\textsuperscript{20,24} from the Landau free-energy functional. Though different in the details, the two limits exhibit an inflection point in $I_Q(H)$. The staggered magnetization remains finite until $H_c$, when the primary order parameter is suppressed to zero. The ordered moments are, however, substantially reduced compared to its zero-field value at significantly smaller magnetic field. Indeed, expanding Eqs. (31) and (32) to the first order in $H^2$ we obtain

$$\frac{m_s^2(H)}{m_s^2(0)} \approx 1 - H^2 \left( \frac{1}{H_c^2} + \frac{12 \mu^2 \Delta}{(\Delta - \Delta_c)(\Delta + 2 \mu^2 \mathcal{J}_0)^2} \right).$$ \hfill (33)

For the completeness we also note that the ferromagnetic component of the induced magnetic moments is given by

$$m_0 = \frac{\mu H}{\Delta + 2 \mu^2 \mathcal{J}_0}.$$ \hfill (34)

for fields smaller than $H^* = (\Delta + 2 \mu^2 \mathcal{J}_0)/2 \mu$. Above this field the ferromagnetic component remains constant until a metamagnetic transition related to a crossing with higher energy crystal-field levels. The uniform component of the induced moments $m_0$ should be measurable from a magnetic contribution to the nuclear Bragg peaks.

C. Finite Fields: Energy Spectrum

We start with the case $H \neq 0, H_s = 0$, since an effective $H_s$ in URu$_2$Si$_2$ should be quite small. Partial polarization of magnetic moments (pseudo-spins) along $\hat{z}$ ($\hat{x}$) axis is taken into account by rotation of pseudo-spins from a laboratory frame to a local (primed) frame:

$$S_i^x = S_i^{x'} \cos \varphi + S_i^{y'} \sin \varphi, \quad S_i^z = -S_i^{x'} \sin \varphi + S_i^{y'} \cos \varphi.$$ \hfill (35)

In the transformed frame and omitting primes the Hamiltonian (14) takes the following form:

$$\hat{H} = 4 \mu^2 \sum_{(i,j)} \mathcal{J}_{ij} \left[ S_i^x S_j^x \cos^2 \varphi + S_i^y S_j^y \sin^2 \varphi + S_i^x S_j^y \sin \varphi \cos \varphi \right.$$  
$$+ (S_i^x S_j^y + S_i^y S_j^x) \sin \varphi \cos \varphi \right]$$

$$- \sum_i \left[ (\Delta \cos \varphi + 2 \mu H \sin \varphi) S_i^z + (2 \mu H \cos \varphi - \Delta \sin \varphi) S_i^x \right].$$ \hfill (36)
The boson representation of the pseudo-spin operators is applied to the above Hamiltonian and the rotation angle \( \varphi \) is determined from the condition of vanishing linear terms in \( a_i \) and \( a_i^\dagger \):

\[
\Delta \tan \varphi + 2\mu^2 J_0 \sin \varphi = 2\mu H .
\]

(37)

At small fields \( \varphi \approx 2\mu H / (\Delta + 2\mu^2 J_0) \).

The harmonic part of the Hamiltonian after the Fourier transformation becomes

\[
\hat{H}_2 = \sum_k a_k^\dagger a_k \Delta \cos \varphi + 2\mu H \sin \varphi - 2\mu^2 \sin^2 \varphi J_0 \\
+ \mu^2 \cos^2 \varphi J_0 + \frac{1}{2} \mu^2 \cos^2 \varphi J_0 (a_k a_{-k} + a_k^\dagger a_{-k}^\dagger). \quad (38)
\]

The \( k \)-independent term is simplified with the help of Eq. (37) to \( \Delta / \cos \varphi \) and after applying the Bogoliubov transformation we obtain the following field dependence of the exciton spectrum:

\[
\omega_k^2 = \frac{\Delta^2}{\cos^2 \varphi} + 2\mu^2 J_0 \Delta \cos \varphi.
\]

(39)

The gap at \( k = Q \) increases quadratically with magnetic field:

\[
\Delta^2(H) \approx \Delta(\Delta - \Delta_c) + \frac{2\mu^2 H^2}{(\Delta + 2\mu^2 J_0)^2} \Delta^2(2\Delta + \Delta_c) . \quad (40)
\]

The parabolic law for the field dependence of the gap has recently been measured in neutron scattering experiments. For an arbitrary wave-vector the field dependence of the exciton energy is

\[
\omega_k^2(H) \approx \omega_k^2(0) + \frac{4\mu^2 H^2 \Delta}{(\Delta + 2\mu^2 J_0)^2} [\Delta - \mu^2 J_0] .
\]

(41)

The field dependence changes its sign, i.e., the energy starts to decrease with magnetic field, for the wave-vectors such that \( \mu^2 J_0 > \Delta \). In terms of zero field frequencies this is equivalent to \( \omega_k > \sqrt{3}\Delta \). In the region in the Brillouin zone where \( \omega_k \approx \sqrt{3}\Delta \) the field dependence of the spectrum becomes vanishingly small. Experimentally, a drastic change in the field dependence has been observed between \( k = Q = (1, 0, 0) \) and \( k = (1.4, 0, 0) \). The present theory explains a qualitative difference in the field response of the two types of excitons. Further inelastic neutron measurements on URu_2Si_2 should allow a detailed comparison with our theory and extraction of microscopic parameters from experimental data.

If both staggered and uniform fields are present, the derivation of the spectrum becomes a bit more complicated. One has to explicitly introduce two types of bosons \( a_i \) and \( b_i \) for two antiferromagnetic sublattices and to calculate spectrum in the magnetic Brillouin zone, which is twice smaller than an original lattice Brillouin zone used above. The transformation to local (primed) axes from the laboratory frame is given by

\[
S_i' = S_i e^{Qr} \sin \varphi_i + S_i'^\prime e^{Qr} \cos \varphi_i,
\]

\[
S_i' = -S_i e^{Qr} \sin \varphi_i + S_i'^\prime e^{Qr} \cos \varphi_i.
\]

(42)

where two angles \( \varphi_i = \varphi_1 \) for \( e^{Qr} = 1 \) and \( \varphi_i = \varphi_2 \) for \( e^{Qr} = -1 \) describe different response of the two sublattices. The angles are determined by

\[
\Delta \tan \varphi_1 + 2\mu^2 J_1 \sin \varphi_1 = 2\mu (H_1 + H_2) + 2\mu^2 J_2 \sin \varphi_2,
\]

\[
\Delta \tan \varphi_2 + 2\mu^2 J_1 \sin \varphi_2 = 2\mu (H_1 - H_2) + 2\mu^2 J_2 \sin \varphi_1.
\]

here we defined separate summation of exchange constants over the same \( J_i = \sum_{i,j \in \delta} J(ij) \) and the different sublattices \( J_{ij} = \sum_{i \in \delta A, j \in \delta B} J(ij) \).

Performing the same steps as in the case of \( H_s = 0 \) we in the end find

\[
\omega_k^{\pm 2} = \frac{1}{2} (\omega_{1k}^2 + \omega_{2k}^2) \pm \sqrt{\frac{1}{4} (\omega_{1k}^2 - \omega_{2k}^2)^2 + 4\mu^4 J_{2k}^2 \Delta^2 \cos \varphi_1 \cos \varphi_2 \sin \varphi_1 \cos \varphi_2},
\]

\[
\omega_{1,2k} = \frac{\Delta^2}{\cos^2 \varphi_{1,2}} + 2\mu^2 J_{1k} \Delta \cos \varphi_{1,2}. \quad (43)
\]

Here, the Fourier transforms are given by \( \hat{J}_{1k} = \sum_{i,j \in \delta} J(ij)e^{ikr_{ij}} \) and \( \hat{J}_{2k} = \sum_{i \in \delta A, j \in \delta B} J(ij)e^{ikr_{ij}} \). The characteristic feature of this spectrum is a small jump between two branches of excitations \( \omega_k^+ \) and \( \omega_k^- \) at the magnetic Brillouin zone boundary, where \( J_{2k} = 0 \). In URu_2Si_2 \( (H_s \neq 0) \) such a jump is induced by external magnetic field \( H \sim H_s \) and becomes negligible again for \( H \gg H_s \), when the above expression Eq. (39) is valid.

Finally, let us comment on the longitudinal polarization of magnetic excitons detected experimentally. In the harmonic approximation, the dynamic structure factor \( S \Delta z(r, \tau) = \langle J_i^z(t)J_{i+r}^z(t+\tau) \rangle \) is expressed via pseudo-spin operators as

\[
S \Delta z(r, \tau) \approx 4\mu^2 \cos^2 \varphi \langle S_i^z(t)S_{i+r}^z(t+\tau) \rangle . \quad (44)
\]

In a weakly polarized Van-Vleck paramagnet for \( \Delta \sim \Delta_c \) one has \( \cos \varphi_{1,2} \approx 1 \). Therefore, transverse ‘spin-wave type modes’ in the pseudo-spin representation correspond to longitudinal polarization of magnetic excitons. The omitted terms in Eq. (44), such as \( \langle S_i^zS_{j+r}^z \rangle \) and \( \langle S_i^z \Delta S_{i+r}^z \rangle \), describe a higher energy two-magnon continuum and their interaction with single-particle states. These terms do not modify the conclusion about longitudinal polarization of single-particle excitations. In the opposite limit \( \Delta \ll \Delta_c \) in a phase with large antiferromagnetic moments \( \cos \varphi_{1,2} \rightarrow 0 \), and the longitudinal dynamic structure factor \( S \Delta z(q, \omega) \) does not have contribution from magnetic excitons. This explains why the neutron scattering measurements failed to observe the magnetic excitations above the first-order transition at \( P_M = 5 \) kbar.

V. COMPARISON WITH EXPERIMENT

Theoretical predictions of the above section can be directly compared with the available experimental data. Specifically, let us consider the field dependence of the
The intensities of the magnetic Bragg peak, the metamagnetic transition in URu$_2$Si$_2$ at $H_c \approx 40$ T can be chosen as the critical field for the spin-density wave. The field dependence of the Bragg peak intensity described by Eqs. (31) and (32) is, then, determined by three microscopic parameters: $\Delta$, $\Delta_c$, $\Delta_t = 2\mu^2|J_Q|$, and $2\mu^2|J_0|$. The last two parameters are fixed by using the experimental data from Eq. (32) for the excitation gap $\Delta_g = \sqrt{\Delta(\Delta - \Delta_t)} \approx 1.59$ meV and its dependence on applied magnetic field. In this way we are left with only one free parameter: the crystal-field splitting $\Delta$.

The two theoretical curves for $\Delta = 3$ meV ($\Delta_c = 2.2$ meV and $2\mu^2|J_0| = 1.3$ meV) and $\Delta = 6$ meV ($\Delta_c = 5.57$ meV and $2\mu^2|J_0| = 2.9$ meV) are presented in Fig. 2 together with the experimental data. Both curves exhibit behavior with an inflection point. The larger value of the gap gives better agreement with the experimental results. For $\Delta = 6$ meV the top of the exciton band at $H = 0$ calculated from Eq. (19) corresponds to $\omega_0 \approx 7.3$ meV. The internal staggered field estimated from Eq. (22) in this case is $H_s \approx 0.08$ T, which is indeed much smaller than applied magnetic fields and justifies the used approximations.

If we further increase $\Delta$, the theoretical dependence for $I_Q(H)$ with the above two constraints practically saturates at the position given by $\Delta = 6$ meV curve. Thus, while we can definitely exclude smaller values $\Delta < 6$ meV for the crystal-field level splitting, the larger values $\Delta > 6$ meV are equally possible. For example, for $\Delta = 10$ meV, which has been suggested on the basis of the early neutron scattering measurements, the parameters obtained from the fits are $\Delta_c = 9.7$ meV, $2\mu^2|J_0| = 4.9$ meV, and $\omega_0 \approx 12.2$ meV. At present, there is no agreement on the value of $\omega_0$ between the two groups of inelastic neutron measurements. Additional more precise neutron scattering investigation of URu$_2$Si$_2$ should greatly help to settle this dispute.

VI. CONCLUSIONS

We have presented a theoretical model to describe unusual magnetism in URu$_2$Si$_2$ below $T_m = 17.5$ K, which combines tiny ordered moments $\mu \sim 0.03\mu_B$ with a large specific heat anomaly at the transition point. At ambient pressure, the transition is driven by an SDW instability in the itinerant subsystem, which also induces weak ordering of local moments on uranium sites. We argue that such a low-$T_c$ spin-density wave has a small form-factor and does not contribute significantly to the neutron scattering, which essentially probe the localized subsystem. Phenomenologically, the phase diagram of URu$_2$Si$_2$ is described by the two order parameter functional, which is consistent with the first-order transition into a state with large antiferromagnetic moments. The microscopic origin of a strong repulsion between two order parameters of the same symmetry needs further clarification. In our view such a behavior may result from a strong renormalization of the RKKY type interaction between the local moments against a rather large SDW gap, which opens over a half of the Fermi surface.

In our discussion we have assumed following the previous works that uranium ions are in the $^3H_4$ ground state. The validity of such an assumption needs further clarification. Also, the high field behavior with an itinerant electron metamagnetic transition would be an interesting test for the dual model and its extension suggested in in the present work. Another open question is temperature evolution of the crystal-field excitations. We believe that the experimentally observed disappearance of the magnetic excitons above the transition temperature is largely related to the closeness of two energy scales: $T_m = 17.5$ K and $\Delta_0 = 1.6$ meV.

The analysis presented in section IVa may be also relevant to UPt$_3$, another heavy-fermion compound with tiny antiferromagnetic moments, for review see Ref. 49. This material does not have apparent anomalies in thermodynamic and kinetic properties at $T_m \approx 5$ K, though the neutron diffraction experiments have detected small antiferromagnetic moments $\mu \sim 0.02\mu_B$. In a possible scenario for UPT$_3$, there is no a SDW instability in the conduction subsystem. The phase transition is driven by the RKKY or the superexchange interaction between local moments, which only slightly exceeds the critical value for zero-temperature antiferromagnetic ordering determined by a crystal-field level splitting. While the crystal level structure is not precisely known for UPT$_3$, the estimates for the specific heat anomaly given in the end of section IVa should be generally valid. Thus, the small ordered antiferromagnetic moments can be reconciled with the absence of large anomalies at the transition point. The pressure effect on antiferromagnetic ordering in UPT$_3$ also agrees with Eqs. (13) and (20), which predict a much faster square-root suppression of zero-
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