Theoretical description of spin-density waves in heavy-fermion systems

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Taking into account intersite f-electron interactions, we present a theoretical model which accounts for the appearance of a possible spin-density wave in heavy-fermion systems. We discuss the characteristics of such a description for all Bravais lattices.

Recent neutron diffraction measurements[1] have indicated the possibility of spin-density-wave (SDW) itinerant antiferromagnetism in some[2] heavy-fermion (HF) systems,[3] the existence of which is strongly claimed by other experimental data[4] too. While much attention has been focused upon the superconducting properties of HF materials, up to now no theoretical model has been developed to account for the emergence of the SDW ordering in the above-mentioned systems. In this Brief Report we attempt to remedy this.

We have to point out that the magnetic state which comes into being in these cases differs from the classical SDW phase:[5,6] The specific heat (C_p) well below the transition temperature (T_N) has a T^3 form[2] and the gap in certain crystallographic directions must still be zero at $T=0$.[7] The large C_p jump at T_N (Ref. 2) (of the same magnitude as in the HF superconductors) is a sign showing that the heavy f electrons are responsible for the magnetic properties in the studied materials. Thus, using our model as a starting point, we take into account a narrow heavy-electron band, the microscopic description of which originates[8,9] in the Kondo lattice:

$$H_1=-\tfrac{1}{2}\sum_{ij\sigma}(ta_{i\sigma}^{\dagger}a_{j\sigma}+\text{H.c.})-\mu\sum_{i\sigma}a_{i\sigma}^{\dagger}a_{i\sigma}+\tfrac{1}{2}\sum_{i\sigma}Ua_{i\sigma}^{\dagger}a_{i\sigma}a_{i-\sigma}^{\dagger}a_{i-\sigma}\ , \tag{1}$$

where i and j denote the nearest-neighbor (NN) sites, $t=2T_K/\pi z$ with T_K as the Kondo temperature, and z the number of NN sites. The last term represents the T_K-dependent on-site repulsion between the heavy electrons. The single-particle energy ξ_k is connected to the Fourier transformation of the first two components of H_1, $\xi_k=\epsilon_k-\mu$, where $\epsilon_k=-t\gamma(k)$, and μ is the chemical potential. $\gamma(k)$ is defined as a sum over the NN site positions R_δ: $\gamma(k)=\sum_\delta\exp(i\mathbf{k}\cdot\mathbf{R}_\delta)$. In a study of the SDW phase the spin-dependent interactions between the NN sites are of great importance. These are connected to the strong k dependence of the gap, because of which the pairing must be intersite in origin.[10] For the SDW phase these contributions may have different nonphononic origins (see Refs. 11–13) as we will discuss later on. We have come to the conclusion that the following Hamiltonian terms greatly contribute to a possible SDW state:

$$H_2=\tfrac{1}{2}\sum_{ij\sigma}Va_{i\sigma}^{\dagger}a_{i\sigma}a_{j\sigma}^{\dagger}a_{j\sigma}-\tfrac{1}{2}\sum_{ij\sigma}Ja_{i\sigma}^{\dagger}a_{i\sigma}a_{j-\sigma}^{\dagger}a_{j-\sigma}-\tfrac{1}{2}\sum_{ij\sigma}Ia_{i\sigma}^{\dagger}a_{j-\sigma}a_{i-\sigma}^{\dagger}a_{j\sigma}\ . \tag{2}$$

The first two terms from H_2 were tested some years ago[14] in a description of an SDW state, and the second term has already been successfully used in the explanation of the $1/T_1$ relaxation rate in HF superconductors.[15] Such terms can be deduced taking into account (i) virtual transitions to the excluded doubly occupied states in the limit of large on-site repulsion and treating the hopping term as a perturbation,[11] and (ii) the exchange of the virtual electron-hole pairs with use of the Schrieffer-Wolf transformation for an extended periodic Anderson model in which Coulomb scattering terms are also taken into account.[12] The last term from H_2 has a phenomenological character at this stage but, as will be seen later on, the introduction of such a term is necessary if we want to take into account stable odd-k-dependent gap functions for Bravais lattices. In order to see the effects of the electron-phonon interaction, we also take into consideration, in a Hamiltonian term H_3, the phononic contributions described by the g_1, g_2, and g_3 coupling constants (in our notation $\tilde{g}_i$) in Eq. (8) from Ref. 8. The Hamiltonian we use is $H_1+H_2+H_3$. For simplicity we neglect the spin-orbit coupling.

It is known[6] that to have a SDW phase appear, there must be a $\mathbf{Q}$ value for which the nesting property has to be satisfied. Since it is assumed that one rare-earth or actinide atom supplies one virtual bound state each, the heavy-electron band is half filled. Under these conditions we analyze at first (in the case of all Bravais lattices) the nesting property for half-filled bands. The relation which must be satisfied in this case is

$$\sum_\delta[1+\exp(i\mathbf{Q}\cdot\mathbf{R}_\delta)]\exp(i\mathbf{k}\cdot\mathbf{R}_\delta)=0\ . \tag{3}$$

If, for a given $\mathbf{Q}$, Eq. (3) is satisfied for any k, then we have a perfect nesting along the whole Fermi surface (FS) and thus the SDW can open a gap along the entire FS. In six cases such a $\mathbf{Q}$ can be obtained for any lattice parameter, e.g., $\mathbf{Q}=\mathbf{i}\pi/a+\mathbf{j}\pi/a+\mathbf{k}\pi/a$ for simple cubic (sc), $\mathbf{Q}=2\mathbf{i}\pi/a+2\mathbf{j}\pi/a+2\mathbf{k}\pi/a$, for base-centered cubic (bcc), etc. (The other four cases are the orthorhombic P and C, the tetragonal, and monoclinic P.) For hexagonal, trigonal, face-centered cubic (fcc), and face-centered orthorhombic lattices, Eq. (3) is satisfied only for fixed k directions which define regions of the FS where nesting occurs and where the SDW gap appears (e.g., $\mathbf{Q}=\pm\mathbf{i}\pi/\sqrt{3}a+\mathbf{j}\pi/a+\mathbf{k}\pi/c$ at $k_y\mp\sqrt{3}k_x=\pi/a$ for the hexagonal case). In the cases of base-centered tetragonal (bct), base-centered orthorhombic, and base-centered monoclinic, nesting can be obtained for the whole FS, or along

fixed k directions, depending on the lattice parameters. For example, in the bct case nesting on the entire FS occurs only if $c/\sqrt{2} < a < \sqrt{3}c/\sqrt{2}$, i.e., $\mathbf{Q} = \mathbf{i}\pi/a + \mathbf{j}\pi/a + \mathbf{k}\pi/c$. The results for the triclinic system are strongly dependent on lattice parameters. That is why we do not give them here. In every situation where not all the FS is opened by the SDW gap, the $\sum_k$ sum must be taken only for the regions which satisfy the nesting.[16,17] The nesting is satisfied even if the band is not half-filled. For example, if at $\mu = 0$ the nesting is satisfied for a $\mathbf{Q}_0$, and applying

$$\gamma(k+k') + \gamma(k-k') = 2\gamma(k) + 0(|k'|^2)$$

for $|k'| \ll 1$, it can be demonstrated that for a small $\mu \neq 0$ the nesting is satisfied as well ($\xi_{k\pm Q} = -\xi_k$). But in this case we have $\mathbf{Q} = \mathbf{Q}_0 - 2\mathbf{k}_\mu$, where $\mathbf{k}_\mu$ represents the variation of $\mathbf{k}_F$ at the nesting points.

In the following, we suppose that the nesting is satisfied at least for a given $\mathbf{Q}$ value and a given direction in the k space. Because we are interested in a possible SDW phase, we neglect other types of ordering within the system. Under these conditions and using the average $\zeta^\sigma(k) = \langle a^\dagger_{k,\sigma} a_{k+Q,\sigma} \rangle$, the effective Hamiltonian and the SDW gap $\Delta_S(k)$ become

$$H_{\text{eff}} = \sum_{k,\sigma} \xi_k a^\dagger_{k,\sigma} a_{k,\sigma} + \frac{1}{2N} \sum_{k,k',\sigma} [g_S(k,k') \zeta^\sigma(k') a^\dagger_{k+Q,\sigma} a_{k,\sigma} + \text{H.c.}] , \tag{4}$$

$$\Delta_S(k) = \tfrac{1}{2} \operatorname{Tr}_\sigma \sigma^z \frac{1}{N} \sum_{k'} g_S(k,k') \zeta^\sigma(k') , \tag{5}$$

where

$$g_S(k,k') = g_0 + \tfrac{1}{2}(g_1+g_2)\gamma(k-k') + \tfrac{1}{2}(g_1-g_2)\gamma(k+k') ,$$

with $g_0 = U - \gamma(Q)(V+J+\tilde{g}_1)$, $g_1 = V - \tilde{g}_2 - I$, and $g_2 = V - \tilde{g}_2 + I$. Using standard methods, for $\Delta_S(k)$ we get

$$\Delta_S(k) = \frac{1}{2N} \sum_{k'} g_S(k,k') [\Delta_S(k')/E(k')] \times \tanh[\beta E(k')/2] , \tag{6}$$

where $E(k) = [\xi_k^2 + \Delta_S^2(k)]^{1/2}$. Equation (6) was deduced without any specification concerning the lattice structure, so this equation holds for any lattice structure. If the lattice is specified [through $\gamma(k-k')$] it is possible to analyze with Eq. (6) the concrete k dependence of $\Delta_S(k)$ in a given compound and the concrete properties of a possible SDW phase which could appear. We exemplify this procedure in the situation where the system has inversion symmetry (as in the case of all Bravais lattices). In this case we can write

$$g_S(k,k') = g_0 + 2g_1 \sum_{\delta'} \cos(\mathbf{R}_{\delta'} \cdot \mathbf{k}) \cos(\mathbf{R}_{\delta'} \cdot \mathbf{k}') + 2g_2 \sum_{\delta'} \sin(\mathbf{R}_{\delta'} \cdot \mathbf{k}) \sin(\mathbf{R}_{\delta'} \cdot \mathbf{k}') . \tag{7}$$

δ' now covers half of the NN sites. In Eq. (7) we have two sets of functions $C = \{\cos(\mathbf{R}_{\delta'} \cdot \mathbf{k})\}$ and $S = \{\sin(\mathbf{R}_{\delta'} \cdot \mathbf{k})\}$ which, for any lattice structure, contain linearly independent terms. Because the neighbors reflect the lattice symmetry, C and S represent separately complete symmetrical sets, being invariants under the symmetry operations G_i of the point group G which describes the analyzed lattice. The study of the transformations within C and S which occur under G_i reveals the irreducible representations (γ_j) among which the mentioned sets span their subspace. For example, $\Gamma_C = A_{1g} + E_g$, $\Gamma_S = F_{1u}$ for sc; $\Gamma_C = A_{1g} + F_{2g}$, $\Gamma_S = A_{2u} + F_{1u}$ for bcc; $\Gamma_C = A_{1g} + E_g + F_{2g}$, $\Gamma_S = F_{1u} + F_{2u}$ for fcc; etc., where $\Gamma_j = \sum_j \gamma_j$ represents the reducible representation associated with C or S in G. Now we can obtain symmetrical orthogonal functions F_{γ_j} situated along a fixed irreducible representation γ_j by projecting the components of the C or S set on γ_j. This can be done[18] with idempotent projection operators which represent, in fact, a linear and orthogonal transformation (τ_i) from the C or S set to the $\{F_{\gamma_j}\}$ set. Thus, after a proper normalization, Eq. (7) becomes

$$g_S(k,k') = g_0 + g_1 \sum_j F_{1\gamma_j}(k) F_{1\gamma_j}(k') + g_2 \sum_j F_{2\gamma_j}(k) F_{2\gamma_j}(k') , \tag{8}$$

where $\{F_{1\gamma_j}\} = \tau_1 C$ and $\{F_{2\gamma_j}\} = \tau_2 S$. Using Eq. (8), the gap equation (6) becomes

$$\Delta_j^l = \frac{1}{2N} \sum_k g_l F_{l\gamma_j}(k) [\Delta_S(k)/E(k)] \tanh[\beta E(k)/2] , \tag{9}$$

where $\Delta_S(k) = \sum_{l,j} \Delta_j^l F_{l\gamma_j}(k)$ and $l = 0,1,2$ [$F_{0\gamma_j}(k) = 1$]. We mention that if the lattice does not have inversion symmetry, a similar analysis can be made. But, in this case, the gap is, in general, a complex variable and the even- and odd-k contributions cannot be separated.[19] Further on, some $F_{l\gamma_j}(k)$ expressions are given. For the sc case

$$F_{1A_{1g}} = \sqrt{2}[\cos(ak_x) + \cos(ak_y) + \cos(ak_z)]/\sqrt{3}, \quad F_{1E_g,1} = [\cos ak_x + \cos(ak_y) - 2\cos(ak_z)]/\sqrt{3} ,$$

$$F_{1E_g,2} = \cos(ak_x) - \cos(ak_y), \quad F_{2F_{1u},1} = \sqrt{2}\sin(ak_x), \quad F_{2F_{1u},2} = \sqrt{2}\sin(ak_y) ,$$

and

$$F_{2F_{1u},3} = \sqrt{2}\sin(ak_z) .$$

In the bcc case, for instance,

$$F_{1A_{1g}} = \{\cos[\tfrac{1}{2}a(-k_x+k_y+k_z)] + \cos[\tfrac{1}{2}a(k_x-k_y+k_z)] + \cos[\tfrac{1}{2}a(k_x+k_y-k_z)] + \cos[\tfrac{1}{2}a(k_x+k_y+k_z)]\}/\sqrt{2} ,$$

$$F_{2A_{2u}} = \{\sin[\tfrac{1}{2}a(-k_x+k_y+k_z)] + \sin[\tfrac{1}{2}a(k_x-k_y+k_z)] + \sin[\tfrac{1}{2}a(k_x+k_y-k_z)] - \sin[\tfrac{1}{2}a(k_x+k_y+k_z)]\}/\sqrt{2} .$$

In the hexagonal system, we have

$$F_{1E_{2g},1}=\{\cos[\tfrac{1}{2}a(k_y+\sqrt{3}k_x)]+\cos[\tfrac{1}{2}a(k_y-\sqrt{3}k_x)]-2\cos(ak_y)\}/\sqrt{3}\ ,$$

$$F_{1E_{2g},2}=\cos[\tfrac{1}{2}a(k_y+\sqrt{3}k_x)]-\cos[\tfrac{1}{2}a(k_y-\sqrt{3}k_x)]\ ,$$

$$F_{2E_{1u},1}=\{\sin[\tfrac{1}{2}a(k_y+\sqrt{3}k_x)]+\sin[\tfrac{1}{2}a(k_y-\sqrt{3}k_x)]+2\sin(ak_y)\}/\sqrt{3}\ ,$$

and

$$F_{2E_{1u},2}=\sin[\tfrac{1}{2}a(k_y+\sqrt{3}k_x)]-\sin[\tfrac{1}{2}a(k_y-\sqrt{3}k_x)]\ .$$

In view of the gap equation (9), the phase diagram (PD) can be constructed. In order to make an energetic stability analysis too, we must obtain the expression of the free energy (F). For the case in which Eq. (6) can be reduced to Eq. (9), following Leggett,[20] one has

$$F=F_0+\sum_1(\Delta_j^1)^2/g_1-\frac{2}{\beta N}\sum_k\ln\{\cosh[\beta E(k)/2]/\cosh(\beta\xi_k/2)\}\ , \tag{10}$$

where F_0 is the free energy of the paramagnetic state. We exemplify the results for the sc lattice at $T=0$ (see Fig. 1). In this case we have $g_0=U+6(V+J+\tilde{g}_1)$ and we use the notation $\tilde{V}=V-\tilde{g}_2$. As can be seen, the importance of the phononic contributions is greatly ($\tilde{g}_1,\tilde{g}_2$) or totally ($\tilde{g}_3$) diminished. The PD contains three energetically stable phases: $\Delta_0\neq0$; $\tilde{\Delta}_4\neq0$; and $\Delta_2\neq0$, $\Delta_3\neq0$, respectively. The notations corresponding to Eq. (9) are $\Delta_0=\Delta_0^0$, $\Delta_1=\Delta_{A_{1g}}^1$, $\Delta_2=\Delta_{E_g,2}^1$, $\Delta_3=\Delta_{E_g,1}^1$, and

$$\Delta_4=\sqrt{2}\,[\Delta^2_{F_{1u},x}\sin(ak_x)+\Delta^2_{F_{1u},y}\sin(ak_y)+\Delta^2_{F_{1u},z}\sin(ak_z)]\ .$$

We denoted by $\tilde{\Delta}_4$ the vector $(\Delta^2_{F_{1u},x},\ \Delta^2_{F_{1u},y},\ \Delta^2_{F_{1u},z})$. We looked for all solutions of the coupled gap equation (9). The results show that in agreement with Balian and Werthamer[21] mixed Δ_j^1 terms cannot appear unrestricted in the stable phase due to the differences which exist between the symmetry of the $F_{1\gamma_j}(k)$ terms. We have to mention that an unstable phase appears for $\tilde{V}/t>6$, i.e., $\Delta_1\neq0$, but this is unstabilized by the Δ_2,Δ_3 phase. For $T\neq0$ in the PD a paramagnetic domain appears around the I/t axis, the volume of which increases with temperature. For the other lattice structures the qualitative image of the PD remains unchanged. In every case the increase of I favors the presence of odd-k-gap solutions, while its decrease allows for the appearance of the stable classical Fedders and Martin-type (Δ_0^0) and even k-dependent order parameters. The competition between these two possible solutions is determined by the g_0/g_1 ratio. As far as the coupling constants from H_2 are concerned, the neutron diffraction data[1] suggest a great V contribution. In the materials studied so far the value of I is estimated to be small. Under these conditions, for any Bravais lattice structure, an even-k-dependent stable gap formation become favorable, analogous to the Δ_2,Δ_3 phase from the sc system. Considering the C_p of these phases, we mention that for the general expression we obtain Eq. (6.1) from Ref. 20. For $T\to0$, the contribution of $dE(k)/d\beta$ is negligible. Considering the sc case with the integral variable transformation $x=\beta\cos(ak_x)$, $y=\beta\cos(ak_y)$, and $z=\beta\cos(ak_z)$, and using a T power-series expansion, for $T\to0$ we get

$$C_p(T)=(T^3/2\pi^3)\int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dy\int_{-\infty}^{+\infty}dz\,E^2\cosh^{-2}(E/2)+0(T^5)\ , \tag{11}$$

where

$$E^2=4t^2(x+y+z)^2+\Delta_2^2(T=0)(x-y)^2$$
$$+\Delta_3^2(T=0)(x+y-2z)^2/3\ .$$

The T^3 dependence of C_p is characteristic not only for the sc lattice. It is determined[22] by the fact that the gap vanishes on points on the FS, and thus it has a more general character. Analogous transformations of that which determines x, y, and z in the sc case can also be determined in all the other cases, where the gap has even k dependence. {For instance, in the hexagonal system, for the $\mathbf{Q}=2\mathbf{j}\pi/a+\mathbf{k}\pi/a$ case, the proper transformation is $x=\beta\cos[\frac{1}{2}a(k_y-\sqrt{3}k_x)]$, $y=\beta\cos[\frac{1}{2}a(k_y+\sqrt{3}k_x)]$, and $z=\beta\cos(ck_z)$. In the bcc lattice we can use $x=\beta\times\cos[\frac{1}{2}a(-k_x+k_y+k_z)]$, $y=\beta\cos[\frac{1}{2}a(k_x-k_y+k_z)]$, and $z=\beta\cos[\frac{1}{2}a(k_x+k_y-k_z)]$.}

In conclusion, the presented model shows that itinerant antiferromagnetism can appear in HF systems. Depending on the coupling constants, this magnetic long-range

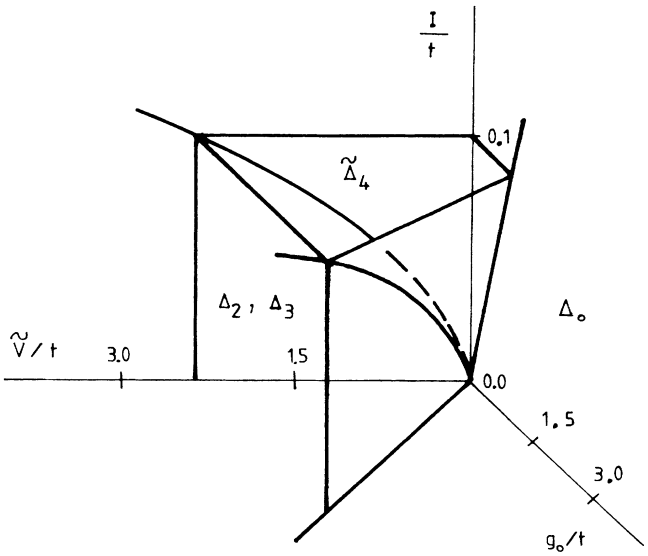

FIG. 1. The phase diagram at $T=0$.

order may have a k-dependent gap which reflects the symmetry of the lattice, a property which cannot be obtained within the classical[5,6] SDW description. The results are in agreement with the experimental measurements and thus the model represents a possible explanation of the magnetism in some HF materials. But we must mention that the presented description is a simple one. It neglects the spin-orbit coupling and considers for the gap equation (6) only those cases where the lattice has inversion symmetry. These situations must be analyzed in the future.

Note added in proof. The detailed analysis of the SDW phase for the simple cubic system is given in Ref. 23.

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