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Spin- and charge-density-wave instabilities in heavy-fermion systems

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Abstract. Spin- and charge-density-wave (SDW, CDW) instabilities are formulated starting from the one-dimensional Anderson lattice model by deriving microscopic gap equations. In the infinite-U case, we show that SDW phase does not appear but CDW may occur. The reason for this difference is that the physical meaning of the slave-boson fluctuation is the fluctuation of charge. In order to incorporate spin fluctuations, application of the 'finite-U' slave-boson technique is proposed. Qualitative features of SDW phase described by the second-order gap equation are discussed.

1. Introduction

One of the main topics of interest in research on heavy-fermion systems (Stewart 1984) is how the grand states at lower temperatures, namely, Fermi liquid states, superconductivity and magnetic instabilities, are realised.

Experimentally, the ground states of Ce heavy-fermion systems were classified in the following way: normal Fermi liquid states, for example, in $CeAl_3$ (Andres *et al* 1975) and $CeCu_6$ (Stewart *et al* 1984); exotic superconductivity in $CeCu_2Si_2$ (Steglich *et al* 1979); and antiferromagnetic ordered states, for instance, in $CeAl_2$ (Barbara *et al* 1977). However, Barth *et al* (1987) found that $CeAl_3$ displays a weak magnetic ordering at temperatures lower than $T_N = 1.2$ K in a muon spin-resonance (μSR) experiment. The effective moment is estimated as at most $0.3\,\mu_B$ and this may be due to an incommensurate spin-density wave (SDW) state. Also, a doping effect on $CeCu_6$ (Gangopadhyay *et al* 1988) induces antiferromagnetic ordering. Then, heavy Fermi liquid states are very close to magnetic ordered states. This property is also found in the superconductor $CeCu_2Si_2$ (Onuki and Komatsubara 1988, Uemura *et al* 1989); exotic superconductivity and antiferromagnetic ordering are found to coexist at temperatures lower than 0.6 K. Material-independent properties of the antiferromagnetism in Ce compounds are that the magnitude of the magnetic moment is extraordinarily small (of the order of $0.1\,\mu_B$) and that the Néel point has the value $T_N \sim 1$ K. The magnetism occurs in the coherent Kondo state. The magnitude of T_N is lower than the Kondo temperature T_K.

Theoretical efforts to understand these properties are only at the initial stage. For instance, the coexistence of anisotropic superconductivity and SDW (Kato and Machida 1987) is analysed based upon the two-dimensional Hubbard model. Ferromagnetism (Cox 1987) is discussed in the molecular-field approximation for the classical 4f-spins. An

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effective interaction between 4f-electrons due to the slave-boson fluctuation (Doniach 1987) is proposed to explain the antiferromagnetism. Competition between the Kondo effect and the RKKY interaction in Kondo lattices is studied and compared with the experiment (Yamamoto and Ohkawa 1988).

The purpose of the present paper is to formulate the $2k_F$-instabilities of heavy-fermion systems in a microscopic manner. The model is the one-dimensional infinite-U Anderson lattice by the slave-boson method (Coleman 1984, Read and Newns 1984). Real materials are three-dimensional. However, $2k_F$-instabilities can be easily formulated by the one-dimensional model. Discussions about this model are expected to give some insight into the physics of heavy-fermion systems. The interaction is mediated by the fluctuation of the slave boson around the mean-field value, which has been proposed in the pioneering work by Doniach (1987). He has derived an effective Hamiltonian due to the fourth-order interactions. In this paper, we derive microscopic gap equations in a diagrammatic way. The two-wave approximation is adopted. It is shown that the SDW state does not occur in our theory, in contrast to Doniach's. However, the charge-density-wave (CDW) instability may occur. The reason for this contradiction is that the Bose fluctuation does not induce a spin fluctuation. The physical meaning of the fluctuation is the fluctuation of charge. The properties of the CDW state due to this interaction are discussed. Further, we propose to use the 'finite-U' slave-boson method (Zou and Anderson 1988), which has been formulated for high-T_c superconductors, in order that we treat spin fluctuations for the description of the SDW phase. Qualitative features of the SDW are discussed.

In the following section, the mean-field theory is reviewed and interaction between heavy fermions is explained. In § 3, we derive a gap equation for SDW and show that the mechanism of Doniach is not applicable. Section 4 is devoted to CDW instability due to the fluctuation. In § 5, we propose to use the 'finite-U' slave-boson method to formulate the SDW. We summarise the paper in § 6.

2. Interactions among heavy quasi-particles in the infinite-U Anderson lattice

We start from the one-dimensional infinite-U Anderson lattice model and make use of the slave-boson technique (Coleman 1984). The Hamiltonian is given by

$$\mathcal{H} = \sum_{i\sigma} (-E_f) f^\dagger_{i\sigma} f_{i\sigma} + \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + V \sum_{i\sigma} (b^\dagger_i c^\dagger_{i\sigma} f_{i\sigma} + f^\dagger_{i\sigma} c_{i\sigma} b_i) + \sum_i \lambda_i \left(\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} + b^\dagger_i b_i - 1 \right) \tag{2.1}$$

where $f_{i\sigma}$ is an operator that annihilates a 4f-electron with spin σ at the ith lattice site whose atomic level has energy $-E_f$. The quantity E_f is taken to be positive. The variable $c_{k\sigma}$ is an annihilation operator of a conduction electron with wavenumber k and spin σ. For simplicity, it is assumed that the conduction electron orbitals have the same magnitude of spin σ as that of the 4f-electrons. The density of states per site of the conduction band is assumed to be constant as $\rho = 1/2D$ at $-D < \varepsilon_k < D$ and zero elsewhere; the dispersion relation is defined as

$$\varepsilon_k = -D + 2D|k|/k_D$$

where k_D is the maximum value of the wavenumber. We define $c_{i\sigma}$ by the relation

$$c_{i\sigma} = N^{-1/2} \sum_k \exp(\mathrm{i}kR_i) c_{k\sigma}.$$

Possible anisotropy in the mixing strength V is not considered. The operator b_i annihilates a slave boson at the ith site. It is introduced to exclude the possibility that two or more electrons occupy the 4f-orbitals of the ith site. The constraints

$$\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} + b^\dagger_i b_i = 1 \tag{2.2}$$

are imposed for each i. They are taken into account in the Hamiltonian (2.1) with Lagrange multiplier λ_i. Since we study only the solutions in which λ_i is site-independent, we put

$$\lambda_i = \lambda \qquad \text{for all } i. \tag{2.3}$$

We assume the Fermi level is $\mu = 0$ so that T_K does not depend on temperature:

$$T_K = D \exp(-DE_f/V^2).$$

The mean-field theory (Read and Newns 1984) assumes the Bose condensation of the slave boson. The *ansatz* is

$$\langle b^\dagger_i \rangle_{\mathrm{mf}} = \langle b_i \rangle_{\mathrm{mf}} = r \qquad \text{for all } i. \tag{2.4}$$

The meaning of the mean field r is that the charge fluctuation is ineffective at low temperatures in heavy-fermion systems in the first approximation. The mean-field theory successfully explains the experimental situations quantitatively: for example, universal behaviours in the specific heat susceptibility, and resistivity (Auerbach and Levin 1986a, b); elastic anomalies (Thalmeier 1987) at low temperatures. We treat the heavy quasi-particles described by the mean-field approximation.

The mean-field parameters, r and λ, are determined by two coupled equations (Read and Newns 1984). One is the self-consistency condition:

$$\frac{V^2}{D} \int_{-D}^{D} \mathrm{d}\varepsilon_k \frac{f(E_+(k)) - f(E_-(k))}{E_+(k) - E_-(k)} + \lambda = 0. \tag{2.5}$$

The other is the constraint equation (2.2):

$$\frac{1}{D} \int_{-D}^{D} \mathrm{d}\varepsilon_k \sum_{\tau=\pm} \left(f(E_\tau(k)) \frac{E_\tau(k) - \varepsilon_k}{E_\tau(k) - E_{-\tau}(k)} \right) + r^2 = 1. \tag{2.6}$$

Here, we denote the dispersion relations of the upper and lower band electrons as $E_+(k)$ and $E_-(k)$, respectively. They are given by

$$E_\pm(k) = \tfrac{1}{2}\{\tilde{E}_f + \varepsilon_k \pm [(\tilde{E}_f - \varepsilon_k)^2 + 4r^2V^2]^{1/2}\} \tag{2.7}$$

where $\tilde{E}_f = -E_f + \lambda$. We have denoted the Fermi function as

$$f(x) = 1/[\exp(x/T) + 1].$$

Solutions of equations (2.5) and (2.6) have the magnitudes $r^2 \simeq DT_K/V^2$ and $\tilde{E}_f \simeq T_K$ at $T = 0$ K (Read and Newns 1984). The mass enhancement factor is

$$m^*/m = \{[\partial E_-(k)/\partial \varepsilon_k]|_{E_-(k)=0}\}^{-1} \simeq D/T_K.$$

The number of electrons is less than 2, which means that the Fermi level crosses the lower band. The Fermi wavenumber is given by

$$k_F = \tfrac{1}{2}k_D(1 + r^2V^2/D\tilde{E}_f) \tag{2.8}$$

which is incommensurate with the lattice in general.

As we discuss the $2k_F$-instabilities in heavy-fermion systems at low temperatures, it is sufficient to reserve the contribution of the electrons that fill the lower band and the fluctuation part of the slave boson. Also, we drop the spontaneous creation and annihilation processes of the fluctuation particle, because these processes must not be included in the interactions (Auerbach and Levin 1986a, Millis and Lee 1987). The effective Hamiltonian becomes

$$\mathcal{H}_{\mathrm{eff}} = \sum_{k\sigma} E_-(k) B^\dagger_{k\sigma} B_{k\sigma} + \lambda \sum_k \beta^\dagger_k \beta_k + \frac{V}{N^{1/2}} \sum_{k\sigma} (-u_p v_{k+p})(\beta^\dagger_k B^\dagger_{p\sigma} B_{k+p,\sigma} + B^\dagger_{k+p,\sigma} B_{p\sigma} \beta_k) \tag{2.9}$$

where $B_{k\sigma}$ denotes the annihilation operator of the lower band electrons, which is connected to $f_{k\sigma}$ and $c_{k\sigma}$ by the relation

$$B_{k\sigma} = v_k f_{k\sigma} - u_k c_{k\sigma}.$$

The annihilation operator of the upper band electron is defined as

$$A_{k\sigma} = u_k f_{k\sigma} + v_k c_{k\sigma}.$$

The quantities u_k and v_k are coefficients of the unitary transformation. They have the forms

$$u_k = [E_-(k) - \tilde{E}_f]/[E_-(k) - \tilde{E}_f)^2 + r^2 V^2]^{1/2} \tag{2.10}$$

and

$$v_k = rV/[(E_-(k) - \tilde{E}_f)^2 + r^2 V^2]^{1/2}. \tag{2.11}$$

The operator β_i is the fluctuation component of the slave boson (β-boson), which is defined by $\beta_i = b_i - r$.

We define the annihilation operators of the right- and left-moving electrons as

$$B^{(+)}_k = B_{k+k_F} \qquad \text{for } -k_F < k < k_D - k_F$$

and

$$B^{(-)}_k = B_{k-k_F} \qquad \text{for } -k_D + k_F < k < k_F$$

respectively. The Hamiltonian (2.9) becomes

$$\begin{aligned}\mathcal{H}_{\mathrm{eff}} = &\sum_{k\sigma} [E^{(+)}(k) B^{(+)\dagger}_{k\sigma} B^{(+)}_{k\sigma} + E^{(-)}(k) B^{(-)\dagger}_{k\sigma} B^{(-)}_{k\sigma}] + \lambda \sum_k \beta^\dagger_k \beta_k \\ &+ \frac{V}{N^{1/2}} \sum_{kp\sigma} [(-u^{(+)}_k v^{(+)}_{k+p} B^{(+)\dagger}_{k+p,\sigma} B^{(+)}_{k\sigma} \beta_p - u^{(-)}_k v^{(+)}_{k+p} B^{(+)\dagger}_{k+p,\sigma} B^{(-)}_{k\sigma} \beta_{p+2k_F} \\ &- u^{(+)}_k v^{(-)}_{k+p} B^{(-)\dagger}_{k+p,\sigma} B^{(+)}_{k\sigma} \beta_{p-2k_F} - u^{(-)}_k v^{(-)}_{k+p} B^{(-)\dagger}_{k+p,\sigma} B^{(-)}_{k\sigma} \beta_p) + \mathrm{HC}]\end{aligned} \tag{2.12}$$

where the origin of the wavenumber is at the Fermi level, which implies that $E^{(+)}(k) = E_-(k + k_F)$ and $E^{(-)}(k) = E_-(k - k_F)$; the quantities $u^{(\pm)}_k$ and $v^{(\pm)}_k$ are obtained by replacing $E_-(k)$ with $E^{(\pm)}(k)$ in equations (2.10) and (2.11), respectively.

3. Gap equation for a SDW instability

Doniach (1987) has treated the β-boson–electron interaction as a perturbation and derived an effective Hamiltonian as the result of the fourth-order interactions. He has argued SDW instability depending upon this effective Hamiltonian. The electrons in the internal processes of the interaction are not renormalised by the $2k_F$-interaction. We argue this effect by deriving an SDW gap equation in a diagrammatic method.

In order to formulate the helical SDW state, we define operators of electrons as $C^{(+)}_{k\sigma} = B^{(+)}_{k\sigma}$ and $C^{(-)}_{k\sigma} = B^{(-)}_{k,-\sigma}$. Then, the Hamiltonian (2.12) is decoupled into the following form:

$$\mathscr{H}_{\text{eff}} = \mathscr{H}_0 + \mathscr{H}_{\text{SDW}} \tag{3.1}$$

where

$$\mathscr{H}_0 = \sum_{k\sigma} [E^{(+)}(k) C^{(+)\dagger}_{k\sigma} C^{(+)}_{k\sigma} + E^{(-)}(k) C^{(-)\dagger}_{k\sigma} C^{(-)}_{k\sigma}] + \lambda \sum_k \beta^\dagger_k \beta_k \tag{3.1a}$$

$$\begin{aligned}\mathscr{H}_{\text{SDW}} = \frac{V}{N^{1/2}} \sum_{kp\sigma} [(&- u^{(+)}_k v^{(+)}_{k+p} C^{(+)\dagger}_{k+p,\sigma} C^{(+)}_{k\sigma} \beta_p - u^{(-)}_k v^{(+)}_{k+p} C^{(+)\dagger}_{k+p,\sigma} C^{(-)}_{k,-\sigma} \beta_{p+2k_F} \\ &- u^{(+)}_k v^{(-)}_{k+p} C^{(-)\dagger}_{k+p,\sigma} C^{(+)}_{k-\sigma} \beta_{p-2k_F} - u^{(-)}_k v^{(-)}_{k+p} C^{(-)\dagger}_{k+p,\sigma} C^{(-)}_{k\sigma} \beta_p) + \text{HC}].\end{aligned} \tag{3.1b}$$

Diagonal propagators for non-interacting heavy electrons are defined by

$$G^{++}_\sigma(\tau, k) = -\langle T_\tau C^{(+)}_{k\sigma}(\tau) C^{(+)}_{k\sigma}(0)\rangle \tag{3.2a}$$

and

$$G^{--}_\sigma(\tau, k) = -\langle T_\tau C^{(-)}_{k\sigma}(\tau) C^{(-)\dagger}_{k\sigma}(0)\rangle. \tag{3.2b}$$

Also, we define the non-interacting β-boson propagator as

$$D(\tau, k) = -\langle T_\tau \beta_k(\tau) \beta^\dagger_k(0)\rangle. \tag{3.3}$$

Their Fourier transformations are calculated with the help of equation (3.1a) to be

$$G^{++}_\sigma(\mathrm{i}\omega, k) = 1/[\mathrm{i}\omega - E^{(+)}(k)] \tag{3.4a}$$

$$G^{--}_\sigma(\mathrm{i}\omega, k) = 1/[\mathrm{i}\omega - E^{(-)}(k)] \tag{3.4b}$$

and

$$D(\mathrm{i}\nu) = 1/(\mathrm{i}\nu - \lambda) \tag{3.4c}$$

where ω and ν are odd and even Matsubara frequencies, respectively. As equation (3.4c) does not depend on the momentum, the index of the momentum is dropped.

Helical SDW instability can be formulated by interactions due to $\mathscr{H}_{\text{SDW}}$. We denote perturbed propagators as $\tilde{G}^{\tau\tau'}_\sigma$ ($\tau, \tau' = \pm$). They are defined by the Dyson equations

$$\tilde{G}^{++}_\sigma(\mathrm{i}\omega, k) = G^{++}_\sigma(\mathrm{i}\omega, k) + \tilde{G}^{+-}_\sigma(\mathrm{i}\omega, k) \Sigma^{-+}_\sigma(\mathrm{i}\omega, k) G^{++}_\sigma(\mathrm{i}\omega, k) \tag{3.5a}$$

and

$$\tilde{G}^{+-}_\sigma(\mathrm{i}\omega, k) = \tilde{G}^{++}_\sigma(\mathrm{i}\omega, k) \Sigma^{+-}_\sigma(\mathrm{i}\omega, k) G^{--}_\sigma(\mathrm{i}\omega, k) \tag{3.5b}$$

where Σ^{+-}_σ and Σ^{-+}_σ are the anomalous self-energy parts, which act as order parameters

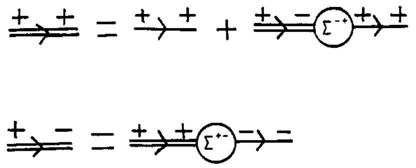

Figure 1. Diagrammatic representation of the Dyson equations (3.5*a*) and (3.5*b*). Single lines represent unrenormalised propagators of electrons. Double lines indicate renormalised propagators.

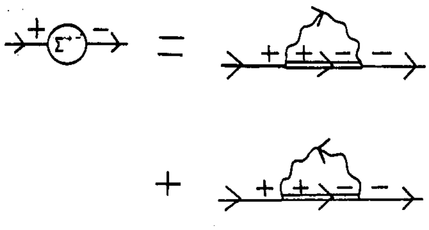

Figure 2. Gap equation of the SDW in the infinite-U case. The wavy line represents the β-boson propagator.

of the SDW. Equations (3.5*a*) and (3.5*b*) are illustrated in figure 1. We approximate Σ_σ^{+-} and Σ_σ^{-+} by the forms of the second-order self-energies where the internal lines of electrons are renormalised. Note that it is needless to consider renormalisation effects on $D(\mathrm{i}\nu)$ at low temperatures $T < T_{\mathrm{K}}$, because the β-boson is massive enough: $\lambda \sim E_{\mathrm{f}} \gg T_{\mathrm{K}}$. The quantity $\Sigma_\sigma^{+-}(\mathrm{i}\omega, k)$ is given by

$$\begin{aligned}\Sigma_\sigma^{+-}(\mathrm{i}\omega,k) = &-V^2 v_k^{(+)} v_k^{(-)} (T/N) \sum_{\mathrm{i}\omega',p} u_p^{(+)} u_p^{(-)} \tilde{G}_\sigma^{+-}(\mathrm{i}\omega',p) D(\mathrm{i}\omega - \mathrm{i}\omega') \\ &- V^2 u_k^{(+)} u_k^{(-)} (T/N) \sum_{\mathrm{i}\omega',p} v_p^{(+)} v_p^{(-)} \tilde{G}_\sigma^{+-}(\mathrm{i}\omega',p) D(\mathrm{i}\omega' - \mathrm{i}\omega). \qquad (3.6)\end{aligned}$$

The structure of equation (3.6) is illustrated in figure 2. We can write down $\Sigma_\sigma^{-+}(\mathrm{i}\omega, k)$ in the same way. Hence, we find that Σ_σ^{+-} and Σ_σ^{-+} have the same form and do not depend on the suffix σ. So, it is convenient to define the notation

$$\Sigma_{\mathrm{A}}(\mathrm{i}\omega, k) = \Sigma_\sigma^{+-}(\mathrm{i}\omega, k) = \Sigma_\sigma^{-+}(\mathrm{i}\omega, k). \qquad (3.7)$$

We perform a static approximation for the β-boson and set $D = 1/(-\lambda)$ in equation (3.6). This is a valid approximation at low temperatures. As the excitation around the Fermi level is important for the $2k_{\mathrm{F}}$-instabilities, it is enough to consider the static order parameter, i.e. $\Sigma_{\mathrm{A}}(k) \equiv \Sigma_{\mathrm{A}}(0, k)$. Equation (3.6) is transformed into

$$\begin{aligned}\Sigma_{\mathrm{A}}(k) = &V^2 v_k^{(+)} v_k^{(-)} \frac{1}{N} \sum_p u_p^{(+)} u_p^{(-)} \frac{\Sigma_{\mathrm{A}}(p)[f(E_1(p)) - f(E_2(p))]}{\lambda[E_1(p) - E_2(p)]} \\ &+ V^2 u_k^{(+)} u_k^{(-)} \frac{1}{N} \sum_p v_p^{(+)} v_p^{(-)} \frac{\Sigma_{\mathrm{A}}(p)[f(E_1(p)) - f(E_2(p))]}{\lambda[E_1(p) - E_2(p)]} \qquad (3.8)\end{aligned}$$

where $E_i(p)$ $(i = 1, 2)$ are solutions of the equation

$$\Sigma_{\mathrm{A}}^2(p) = [\omega - E^{(+)}(p)][\omega - E^{(-)}(p)]$$

and are given by

$$E_{\frac{1}{2}}(p) = \tfrac{1}{2}\{E^{(+)}(p) + E^{(-)}(p) \pm [(E^{(+)}(p) - E^{(-)}(p))^2 + 4\Sigma_{\mathrm{A}}^2(p)]^{1/2}\}. \qquad (3.9)$$

Further, we can simplify equation (3.8) by the effective-mass approximation at the Fermi level:

$$E^{(+)}(k) \simeq 2D(m/m^*)(k/k_{\mathrm{D}})$$

and

$$E^{(-)}(k) \simeq -2D(m/m^*)(k/k_D).$$

We shall approximate coefficients of the unitary transformation by the magnitudes at the Fermi level:

$$u_k^{(\pm)} \simeq -(m/m^*)^{1/2} \qquad \text{and} \qquad v_k^{(\pm)} \simeq (1-m/m^*)^{1/2} \sim 1.$$

The order parameter $\Sigma_A(k)$ is also replaced by the value at $k=0$: $\Delta = \Sigma_A(0)$. Hence, equation (3.8) becomes

$$\Delta = -V^2 \frac{m}{m^*}\frac{1}{k_D}\int_0^{k_c} \mathrm{d}p\, \Delta \tanh\left\{\frac{1}{2T}\left[4D^2\left(\frac{m}{m^*}\frac{p}{k_D}\right)^2 + \Delta^2\right]^{1/2}\right\}$$

$$\times \left\{2\lambda\left[4D^2\left(\frac{m}{m^*}\frac{p}{k_D}\right)^2 + \Delta^2\right]^{1/2}\right\}^{-1} \tag{3.10}$$

where k_c is a cut-off of the momentum. The approximation used in deriving equation (3.10) is intended to retain the essence of the one-dimensional model: effects of the complete nesting of the Fermi surface. A more rigorous numerical treatment of equation (3.8) is not expected to alter the result of this paper.

It is found that the signs of the left- and right-hand sides of equation (3.10) do not agree. Equation (3.10) does not have solutions where $\Delta =\neq 0$. This means that SDW instability does not occur by interactions with the fluctuation. If the internal lines of electrons of the effective interaction of Doniach's model are renormalised, this model does not describe a SDW instability.

4. CDW due to charge fluctuation

One of the $2k_F$-instabilities is a CDW instability. We shall consider the possibility of CDW by the model of equation (2.12). This equation is decoupled into diagonal and interaction parts as

$$\mathcal{H}_{\text{eff}} = \mathcal{H}_0 + \mathcal{H}_{\text{CDW}} \tag{4.1}$$

where

$$\mathcal{H}_0 = \sum_{k\sigma}[E^{(+)}(k)B_{k\sigma}^{(+)\dagger}B_{k\sigma}^{(-)} + E^{(-)}(k)B_{k\sigma}^{(-)\dagger}B_{k\sigma}^{(-)}] + \lambda\sum_k \beta_k^\dagger\beta_k \tag{4.1a}$$

$$\mathcal{H}_{\text{CDW}} = \frac{V}{N^{1/2}}\sum_{kp\sigma}[(-u_k^{(+)}v_{k+p}^{(+)}B_{k+p,\sigma}^{(+)\dagger}B_{k\sigma}^{(+)}\beta_p - u_k^{(-)}v_{k+p}^{(+)}B_{k+p,\sigma}^{(+)\dagger}B_{k\sigma}^{(-)}\beta_{p+2k_F}$$

$$- u_k^{(+)}v_{k+p}^{(-)}B_{k+p,\sigma}^{(-)\dagger}B_{k\sigma}^{(+)}\beta_{p-2k_F} - u_k^{(-)}v_{k+p}^{(-)}B_{k+p,\sigma}^{(-)\dagger}B_{k\sigma}^{(-)\dagger}\beta_p) + \text{HC}]. \tag{4.1b}$$

We define diagonal propagators of electrons as

$$G_\sigma^{++}(\tau,k) = -\langle T_\tau B_{k\sigma}^{(+)}(\tau)B_{k\sigma}^{(+)\dagger}(0)\rangle \tag{4.2a}$$

and

$$G_\sigma^{--}(\tau,k) = -\langle T_\tau B_{k\sigma}^{(-)}(\tau)B_{k\sigma}^{(-)\dagger}(0)\rangle. \tag{4.2b}$$

It is noted that we employ the same notation, G and $\tilde{G}$, in this section as in § 3 for

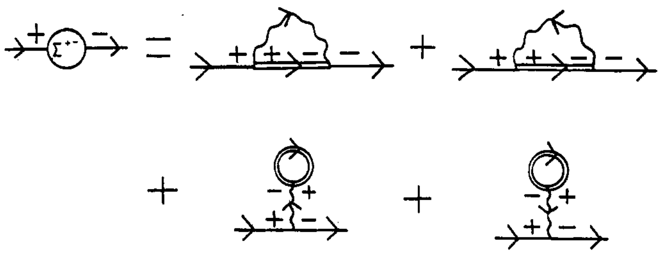

Figure 3. Gap equation of the CDW in the infinite-U case.

convenience, though the definitions are changed. The Dyson equations are the same as equations (3.5a) and (3.5b). The anomalous self-energy part for CDW instability becomes

$$\Sigma^{+-}(\mathrm{i}\omega, k) = -V^2 v_k^{(+)} v_k^{(-)} \frac{T}{N} \sum_{\mathrm{i}\omega', p} u_p^{(+)} u_p^{(-)} \tilde{G}^{+-}(\mathrm{i}\omega', p) D(\mathrm{i}\omega - \mathrm{i}\omega')$$
$$- V^2 u_k^{(+)} u_k^{(-)} \frac{T}{N} \sum_{\mathrm{i}\omega', p} v_p^{(+)} v_p^{(-)} \tilde{G}^{+-}(\mathrm{i}\omega', p) D(\mathrm{i}\omega' - \mathrm{i}\omega)$$
$$+ 2V^2 v_k^{(+)} u_k^{(-)} \frac{T}{N} \sum_{\mathrm{i}\omega', p} u_p^{(+)} v_p^{(-)} \tilde{G}^{+-}(\mathrm{i}\omega', p) D(0)$$
$$+ 2V^2 u_k^{(+)} v_k^{(-)} \frac{T}{N} \sum_{\mathrm{i}\omega', p} v_p^{(+)} u_p^{(-)} \tilde{G}^{+-}(\mathrm{i}\omega', p) D(0). \quad (4.3)$$

A diagrammatic representation of equation (4.3) is given in figure 3. The same simplifications of equation (4.3) as in § 3 give

$$\Delta = 2V^2 \frac{m}{m^*} \frac{1}{k_{\mathrm{D}}} \int_0^{k_{\mathrm{c}}} \mathrm{d}p\, \Delta \tanh\left\{ \frac{1}{2T} \left[4D^2 \left(\frac{m}{m^*} \frac{p}{k_{\mathrm{D}}} \right)^2 + \Delta^2 \right]^{1/2} \right\}$$
$$\times \left\{ 2\lambda \left[4D^2 \left(\frac{m}{m^*} \frac{p}{k_{\mathrm{D}}} \right)^2 + \Delta^2 \right]^{1/2} \right\}^{-1} \quad (4.4)$$

where $\Delta = \Sigma^{+-}(0, 0)$.

Fortunately, solutions exist to equation (4.4). This is due to the difference between equations (3.6) and (4.3). The first and second terms on the right-hand sides are mathematically equivalent. But, there are the third and fourth terms in equation (4.3), which correspond to tadpole diagrams in figure 3. These 'vacuum-fluctuation' contributions overcome the first and second terms to change the minus sign of equation (3.10) into the plus sign of equation (4.4). Originally, the b-boson is attributed to the state where the 4f-electrons do not exist. So, it is obvious that the fluctuation field, namely, the β-boson, mediates charge-fluctuation processes among heavy quasi-particles. This is the physical reason why the SDW instability does not occur but the CDW instability may occur due to the β-boson–electron interactions. Mathematically, the difference is represented by the presence of tadpole diagrams.

Actually, CDW phases have not been experimentally observed yet. But it might be theoretically interesting to see properties of the CDW. Equation (4.4) is transformed into

$$1 = \frac{V^2}{2D\lambda}\int_0^\Lambda \mathrm{d}x \frac{\tanh\{[1/(2T)](x^2+\Delta^2)^{1/2}\}}{(x^2+\Delta^2)^{1/2}} \tag{4.5}$$

where Λ is a cut-off of the energy, $\Lambda \equiv 2D(m/m^*)(k_c/k_D)$; it has a magnitude of the order of T_K. The transition temperature T_c is calculated to be

$$T_c = 1.134\,\Lambda\exp(-2D\lambda/V^2) \sim \Lambda(T_K/D)^2. \tag{4.6}$$

This is much smaller than T_K. It will be difficult to observe this phase transition even if it occurs. We also calculate the order parameter at $T=0$ to obtain $\Delta \simeq 2\Lambda\exp(-2D\lambda/V^2) \sim 2\Lambda(T_K/D)^2$. Then, the ordered charge per site is estimated to be

$$\left|2\frac{T}{N}\sum_{\mathrm{i}\omega,k}\tilde{G}^{+-}(\mathrm{i}\omega,k)\right| \simeq 4\frac{\lambda\Delta}{V^2}\frac{m}{m^*} \sim 8(1-n_f)\frac{T_K}{D}\frac{\lambda\Lambda}{DT_K} \tag{4.7}$$

where n_f is the number of f-electrons per site. The quantity $\lambda\Lambda/DT_K$ may have the order of unity. The charge ordering by the present mechanism is very small.

5. A gap equation of SDW in 'finite-U' Anderson lattice

In previous sections, we have considered the infinite-U Anderson lattice. Interaction among electrons is via charge fluctuation mediated by the β-boson. Spin fluctuation in each lattice site has not been considered in the infinite-U model. However, in real materials, it is expected that spin fluctuation takes part in the dynamics of valence fluctuations. Observation of magnetic order may be the explicit evidence. In this section, we propose to formulate a SDW instability due to spin fluctuation by extending the slave-boson method to a 'finite-U' system. This extension has been performed in the theory of the high-T_c oxide superconductors (Zou and Anderson 1988).

We shall consider the following model:

$$\mathcal{H} = \sum_{i\sigma}(-E_f)f^\dagger_{i\sigma}f_{i\sigma} + \sum_i(-2E_f+U)d^\dagger_i d_i + \sum_{k\sigma}\varepsilon_k c^\dagger_{k\sigma}c_{k\sigma}$$
$$+ V\sum_{i\sigma}[(f^\dagger_{i\sigma}b_i + \sigma d^\dagger_i f_{i,-\sigma})c_{i\sigma} + \mathrm{HC}]$$
$$+ \sum_i\lambda_i\left(\sum_\sigma f^\dagger_{i\sigma}f_{i\sigma} + b^\dagger_i b_i + d^\dagger_i d_i - 1\right) \tag{5.1}$$

where an additional slave boson d_i is introduced to represent the doubly occupied 4f-state at the ith lattice site; the energy of the d-boson is $-2E_f + U$. Accordingly, the form of the mixing interaction is changed. Also, the constraint (2.2) is transformed into

$$\sum_\sigma f^\dagger_{i\sigma}f_{i\sigma} + b^\dagger_i b_i + d^\dagger_i d_i = 1. \tag{5.2}$$

We consider the mean-field approximation for d-bosons. This generates curious unphysical processes from the mixing term: pair annihilation and creation processes of f- and c-electrons of the form

$$V\langle d\rangle \sum_{i\sigma} \sigma(f_{i,-\sigma}c_{i\sigma} + c_{i\sigma}^{\dagger}f_{i,-\sigma}^{\dagger}).$$

The expectation value of this term must be zero. Then, the mean-field free energy is parabolic with respect to $\langle d\rangle$, without linear terms in $\langle d\rangle$. This implies $\langle d\rangle = 0$. We treat the d-boson–electron interactions by explicit perturbations. This may be valid if the mean-field approximation for b-bosons describes well the band structure of heavy fermions. Introducing the mean field r, the value of which does not change from that in previous sections, and performing the two-wave approximation as in § 2, we transform equation (5.1) into the effective Hamiltonian

$$\mathcal{H}_{\text{eff}} = \mathcal{H}_0 + \mathcal{H}_{\text{SDW}} \tag{5.3}$$

where

$$\mathcal{H}_0 = \sum_{k\sigma} [E^{(+)}(k)C_{k\sigma}^{(+)\dagger}C_{k\sigma}^{(+)} + E^{(-)}(k)C_{k\sigma}^{(-)\dagger}C_{k\sigma}^{(-)}] + (-2E_{\text{f}} + U + \lambda)\sum_k d_k^{\dagger}d_k + \lambda\sum_k \beta_k^{\dagger}\beta_k \tag{5.3a}$$

$$\begin{aligned}\mathcal{H}_{\text{SDW}} = \frac{V}{N^{1/2}}\sum_{kp\sigma} [(&-u_k^{(+)}v_{k+p}^{(+)}C_{k+p,\sigma}^{(+)\dagger}C_{k\sigma}^{(+)}\beta_p - u_k^{(-)}v_{k+p}^{(+)}C_{k+p,\sigma}^{(+)\dagger}C_{k,-\sigma}^{(-)}\beta_{p+2k_{\text{F}}} \\ &- u_k^{(+)}v_{k+p}^{(-)}C_{k+p,\sigma}^{(-)\dagger}C_{k,-\sigma}^{(+)}\beta_{p-2k_{\text{F}}} - u_k^{(-)}v_{k+p}^{(-)}C_{k+p,\sigma}^{(-)\dagger}C_{k\sigma}^{(-)}\beta_p) + \text{HC}] \\ &+ \frac{V}{N^{1/2}}\sum_{kp\sigma}\{[-\sigma v_k^{(+)}u_p^{(+)}d_{k+p+2k_{\text{F}}}^{\dagger}C_{k,-\sigma}^{(+)}C_{p\sigma}^{(+)} \\ &+ \sigma(v_k^{(+)}u_p^{(-)} + u_k^{(+)}v_p^{(-)})d_{k+p}^{\dagger}C_{k\sigma}^{(+)}C_{p\sigma}^{(-)} \\ &- \sigma v_k^{(-)}u_p^{(-)}d_{k+p-2k_{\text{F}}}^{\dagger}C_{k\sigma}^{(-)}C_{p,-\sigma}^{(-)}] + \text{HC}\Big\}\end{aligned} \tag{5.3b}$$

where operators $C_{k\sigma}^{(+)} = B_{k\sigma}^{(+)}$ and $C_{k\sigma}^{(-)} = B_{k,-\sigma}^{(-)}$ are introduced in order to consider helical SDW instability. A propagator of the d-boson is defined as

$$D_{\text{d}}(\tau, k) = -\langle T_{\tau}d_k(\tau)d_k^{\dagger}(0)\rangle. \tag{5.4}$$

Its Fourier transform is

$$D_{\text{d}}(\text{i}\nu) = 1/[\text{i}\nu - (-2E_{\text{f}} + U + \lambda)]. \tag{5.5}$$

Definitions of other propagators are the same as in § 3. The gap equation can be derived in a form of the second-order self-energy part. The result is

$$\begin{aligned}\Sigma_{\sigma}^{+-}(\text{i}\omega, k) = &- V^2 v_k^{(+)}v_k^{(-)}\frac{T}{N}\sum_{\text{i}\omega,p} u_p^{(+)}u_p^{(-)}\tilde{G}_{\sigma}^{+-}(\text{i}\omega', p)D(\text{i}\omega - \text{i}\omega') \\ &- V^2 u_k^{(+)}u_k^{(-)}\frac{T}{N}\sum_{\text{i}\omega',p} v_p^{(+)}v_p^{(-)}\tilde{G}_{\sigma}^{+-}(\text{i}\omega', p)D(\text{i}\omega' - \text{i}\omega)\end{aligned}$$

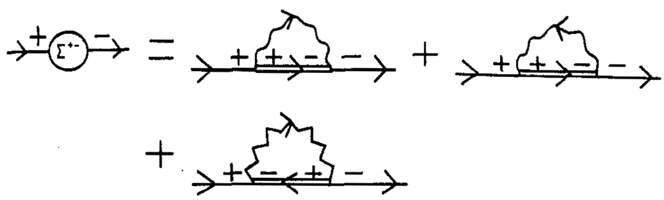

Figure 4. Gap equation of the SDW by the 'finite-U' slave-boson technique. The zigzag line indicates the d-boson propagator D_{d}.

$$+ V^2 \frac{T}{N} \sum_{\mathrm{i}\omega', p} (u_k^{(+)} v_p^{(-)} + v_k^{(+)} u_p^{(-)})(u_p^{(+)} v_k^{(-)} + v_p^{(+)} u_k^{(-)}) \times \tilde{G}_\sigma^{+-}(\mathrm{i}\omega', p) D_{\mathrm{d}}(\mathrm{i}\omega + \mathrm{i}\omega'). \tag{5.6}$$

The corresponding diagram is shown in figure 4. It should be noted that the third term of equation (5.6) contains the fermion loop so that the factor (-1) is multiplied.

Performing the static approximation for β- and d-boson propagators and defining $\Delta \equiv \Sigma_\sigma^{+-}(0, 0)$, we obtain the reduced gap equation

$$\Delta = \left(\frac{2V^2}{U+\lambda-2E_{\mathrm{f}}} - \frac{V^2}{\lambda}\right) \frac{m}{m^*} \frac{1}{k_{\mathrm{D}}} \int_0^{k_{\mathrm{c}}} \mathrm{d}p\, \Delta \tanh\left\{\frac{1}{2T}\left[4D^2\left(\frac{m}{m^*}\frac{p}{k_{\mathrm{D}}}\right)^2 + \Delta^2\right]^{1/2}\right\} \times \left\{2\left[4D^2\left(\frac{m}{m^*}\frac{p}{k_{\mathrm{D}}}\right)^2 + \Delta^2\right]^{1/2}\right\}^{-1} \tag{5.7}$$

The condition that non-zero solutions exist in equation (5.7) is

$$J \equiv \frac{2V^2}{U+\lambda-2E_{\mathrm{f}}} - \frac{V^2}{\lambda} > 0. \tag{5.8}$$

Equation (5.8) is transformed into

$$U < 2E_{\mathrm{f}} + \lambda \simeq 3E_{\mathrm{f}}. \tag{5.9}$$

Then, we find that there is a maximum value for U, below which the SDW occurs in the second-order gap equation. As E_{f} is of the order of D, equation (5.9) may be a not too strong condition.

We estimate properties of the SDW. The transition temperature T_{N} is calculated as in § 4 to be

$$T_{\mathrm{N}} = 1.134\Lambda \exp(-2D/J). \tag{5.10}$$

For example, when $U = \frac{7}{3}E_{\mathrm{f}}$, we obtain $T_{\mathrm{N}} \sim \Lambda(T_{\mathrm{K}}^*/D)$. The quantity T_{K}^* is the Kondo temperature of the finite-U system:

$$T_{\mathrm{K}}^* = D \exp\{-D[(V^2/E_{\mathrm{f}}) - V^2/(U - E_{\mathrm{f}})]^{-1}\}.$$

We expect that the relation $T_{\mathrm{N}} < T_{\mathrm{K}}^*$ holds for general values of U. At $T = 0$, we can calculate the order parameter to obtain $\Delta = 2\Lambda \exp(-2D/J)$. The ordered moment per site is estimated to be

$$M = \left|2\frac{T}{N}\sum_{\mathrm{i}\omega, k} \tilde{G}^{+-}(\mathrm{i}\omega, k)\right| \sim \frac{2\Delta}{J}\frac{m^*}{m} \sim 8(1 - n_{\mathrm{f}}) \frac{\lambda\Lambda}{DT_{\mathrm{K}}^*}\left(\frac{T_{\mathrm{K}}^*}{D}\right)^{3/2} \tag{5.11}$$

when $U = \frac{7}{3}E_{\mathrm{f}}$. Here, the quantity n_{f} is the number of f-electrons per site. As we take the quantity $\lambda\Lambda/DT_{\mathrm{K}}^{*}$ to be of the order of unity, we can say that equation (5.11) might explain the experimental finding that the magnitude of the magnetic moment is very small. Although precise quantitative discussions are not within the scope of our present theory, our results might have something to do with the properties of the antiferromagnetism in heavy-fermion systems that the Néel temperature is very low and the magnetic moment is small.

6. Summary and discussions

We have formulated the $2k_{\mathrm{F}}$-instabilities in heavy-fermion systems starting from the one-dimensional Anderson lattice model by deriving microscopic gap equations. In the infinite-U case, we have shown that the SDW phase does not appear but the CDW may occur. It is pointed out that the reason for the difference is that the slave-boson fluctuation mediates the charge-fluctuation processes physically. In order to formulate the SDW phase, we have proposed to adopt the 'finite-U' slave-boson method. The gap equation has been derived by second-order perturbations. It is found that the SDW phase can appear for a suitable range of parameters. We have considered whether the properties of the SDW, i.e. low Néel temperature and small magnitude of magnetic order, may be understood by our formalism, even if quantitative discussions must await future research.

The drastic conclusion, the absence of the SDW in the infinite-U model, might have come from the one-dimensional nature: possible scattering processes are highly reduced on the limited Fermi surface. This effect strongly separates different ordered phases.

We have treated the heavy quasi-particles by the mean-field approximation. Construction of a theory that does not depend on the mean field is a difficult but important problem. It must be checked whether our qualitative discussions are changed or not. These problems will wait for further research.

We can treat complete nesting of the Fermi surface by one-dimensional models. However, real compounds are three-dimensional. The nesting may not be complete; coexistence of different ordered phases, for example, superconductivity and antiferromagnetism, is reported. It is an interesting problem to extend our theory to the higher-dimensional model and analyse the cross-over between some ordered states due to the incomplete nesting.

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