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One- and two-loop corrections in the periodic Coqblin–Schrieffer model

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Abstract
We investigate the periodic Coqblin–Schrieffer model in terms of functional integral formalism, taking account of one- and two-loop corrections to the mean-field solution. First, we take account of the one-loop (1L) diagrams to determine the order parameter corresponding to the heavy-fermion state for the symmetric case with isotropic hybridization. It is shown that the mean-field order parameter is enhanced by the radial fluctuations, while it is reduced by the phase fluctuations. Therefore, if the phase fluctuations are gauge-fixed by the Anderson–Higgs mechanism, the heavy-fermion state is more stabilized due to the corrections. Second, we give the analytical expressions for the two-loop corrections to the free energy, which consist of the 1L corrections to the fermion self-energy, the boson self-energy, and the fermion–boson vertex function.

In order to describe the heavy-fermion state, we have investigated the periodic Coqblin–Schrieffer (PCS) model by applying the mean-field approximation (MFA) [1] and the one-loop approximation (1LA) [2]. In [1] we have shown that the metamagnetic-like behaviour of $CeRu_2Si_2$ and the non-Fermi-liquid-like behaviour of $CeNi_2Ge_2$ can be described with the same origin of the singularity in the density of quasi-particle states as for the case with anisotropic c–f hybridization. In the MFA, however, there appears a phase transition between the heavy-fermion state and the localized state of f electrons, which has not been observed experimentally. It is therefore of great interest to examine how the transition is modified by corrections to the mean-field solution. For that purpose, we have developed a renormalized perturbation theory employing the functional integral method, part of which has already been reported in [2]. We have examined the self-consistent equation for the order parameter in the 1LA, and shown that, if phase fluctuations are gauge-fixed by the Anderson–Higgs mechanism similarly to the superconductivity [2–4], the heavy-fermion state is more stabilized due to the corrections [2]. In this paper we give the one-loop (1L) contributions to the order parameter from the radial and the phase fluctuations separately and present the analytical expressions for the two-loop corrections to the free energy, which consist of the 1L corrections to the fermion self-energy, the boson self-energy, and the fermion–boson vertex function.

We consider the PCS model:[1, 5]

$$\hat{H} = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} + \sum_{iM} (\varepsilon_{\mathrm{f}} + E_M) \hat{f}^{\dagger}_{iM} \hat{f}_{iM} - J \sum_{iMM'} \hat{f}^{\dagger}_{iM} \hat{c}_{iM} \hat{c}^{\dagger}_{iM'} \hat{f}_{iM'}, \tag{1}$$

where $\hat{c}^{\dagger}_{\vec{k}\sigma}$ ($\hat{c}_{\vec{k}\sigma}$) and $\hat{f}^{\dagger}_{iM}$ ($\hat{f}_{iM}$) are creation (annihilation) operators for a conduction electron in the plane-wave state with wavevector $\vec{k}$ and spin σ and an f electron in the state labelled by M at site i, respectively. ε_{f} is the effective f-level energy, and E_M is the Zeeman term given by $E_M = -g_J \mu_{\mathrm{B}} \langle M|J_z|M\rangle H$ due to the magnetic field H applied along the z-axis. We consider only the lowest Kramers doublet, $|M\rangle$ and $|\bar{M}\rangle$, and neglect the Zeeman term in the conduction electron energy for simplicity. The Fourier transform c_{iM} in the third term of equation (1) is defined as $\hat{c}_{iM} = (1/\sqrt{N}) \sum_{\vec{k}\sigma} v^{*}_{\vec{k}M\sigma} \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{R}_i} \hat{c}_{\vec{k}\sigma}$, where $v_{\vec{k}M\sigma}$ are the normalized mixing matrix elements in the periodic Anderson model, and N the number of f sites.

We calculate the partition function $Z = \mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}$ on the basis of the functional integral technique in which the Fermi operators in equation (1) are replaced by the Fermi fields ($\bar{c}_{\vec{k}\sigma}$, etc). We introduce the auxiliary Bose fields ($\bar{\phi}_i$ and ϕ_i) to decouple the scattering term of equation (1) as

$$-J \sum_{iM} (\bar{\phi}_i \bar{c}_{iM} f_{iM} + \bar{f}_{iM} c_{iM} \phi_i) + J \sum_i |\phi_i|^2.$$

Then, we parametrize the Bose fields as

$$\phi_i = \sigma_0 + (\rho_i + \mathrm{i}\pi_i)/\sqrt{2}, \tag{2}$$

where σ_0 is the mean-field value, and ρ_i and π_i are the radial and the phase components of the fluctuations, respectively. The Fermi fields can be integrated out to give rise to the Helmholtz free energy as

$$F = \mu N_{\mathrm{e}} + J N \sigma_0^2 - k_{\mathrm{B}} T \,\mathrm{tr} \log \hat{G}_0^{-1} + \Delta F, \tag{3}$$

$$\Delta F = -k_{\mathrm{B}} T \log \langle \mathrm{e}^{\mathrm{tr}\log(1+\hat{G}_0 \hat{M}_{\mathrm{f}})} \rangle. \tag{4}$$

Here N_{e} is the total number of the electrons, and $\hat{G}_0$ is a mean-field Green function matrix. Note that the quasiparticle Green function $g_\xi(n)$ is given by $g_\xi(n) = (\mathrm{i}\omega_n - (\omega_\xi - \mu))^{-1}$ whose eigenenergy ω_ξ is given by

$$\omega_\xi = \tfrac{1}{2} \left\{ (\varepsilon_{\vec{k}} + E_M) + \eta \sqrt{(\varepsilon_{\vec{k}} - E_M)^2 + 4 J^2 \sigma_0^2 I_{\vec{k}M}} \right\}, \tag{5}$$

where ξ denotes $(\vec{k}, M, \eta)$ with $\eta = \pm$, and $I_{\vec{k}M} = \sum_\sigma |v_{\vec{k}M\sigma}|^2$. $\hat{M}_{\mathrm{f}}$ is the fluctuation (4×4) matrix without diagonal elements, whose off-diagonal ones are given by $-J v_{\vec{k}+\vec{q}M\sigma} \bar{\phi}_{-\vec{q}}$, etc. The notation $\langle \cdots \rangle$ denotes the functional integrals over the Bose fields which should be performed.

If we expand the factor $\langle \mathrm{e}^{\mathrm{tr}\log(1+\hat{G}_0 \hat{M}_{\mathrm{f}})} \rangle$ in equation (4) in terms of $\hat{G}_0 \hat{M}_{\mathrm{f}}$, we obtain the perturbation expansion for the free energy. The one- and two-loop corrections to the free energy are given as

$$\Delta F^{(1)} = \tfrac{1}{2} k_{\mathrm{B}} T \langle \mathrm{tr}(\hat{G}_0 \hat{M}_{\mathrm{f}})^2 \rangle, \tag{6}$$

$$\Delta F^{(2)} = \tfrac{1}{4} k_{\mathrm{B}} T \{ \langle \mathrm{tr}(\hat{G}_0 \hat{M}_{\mathrm{f}})^4 \rangle - \tfrac{1}{2} \langle \{ \mathrm{tr}(\hat{G}_0 \hat{M}_{\mathrm{f}})^2 \}^2 \rangle \}. \tag{7}$$

The Feynman rules are shown in figure 1. The solid and wavy lines represent the fermion and the boson $\{\rho, \pi\}$-propagators, respectively.

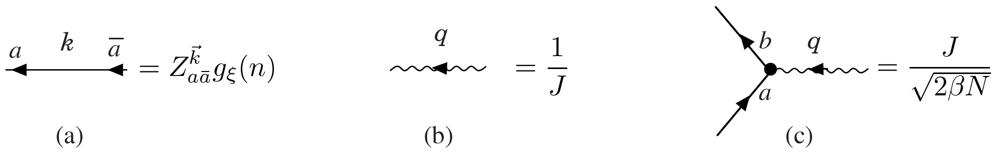

Figure 1. Feynman rules for the propagators and the ϕ-fermion vertex: (a) the fermion propagator; (b) the ρ- and π-propagators; and (c) the $\{\rho, \pi\}$-fermion vertex.

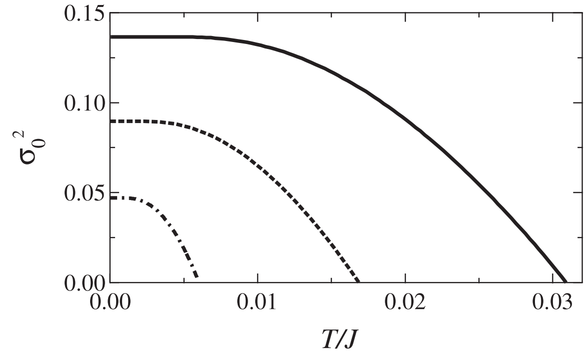

Figure 2. Order parameter σ_0^2 as a function of T for $J/D = 1/6$: the solid curve shows σ_0^2 for the 1L radial fluctuations, the dashed curve that for the MFA, and the dash–dotted curve that for the 1L phase fluctuations.

In the 1LA, the ρ- and the π-fluctuations contribute separately to the free energy; they are given as

$$\Delta F^{(1)}_{\rho,\pi}(\sigma_0) = NJ[1 \mp \tfrac{1}{4}\sigma_0^2 K_M^2(\sigma_0^2)], \tag{8}$$

where $-$ (+) is for the ρ-mode (π-mode), and $K_M(\sigma_0^2) = \sum_{k,\eta} z^{\mathrm{gap}}_{kM}(\omega_\tau) f(\omega_\tau)$ with $z^{\mathrm{gap}}_{kM}(\omega_\tau) = J(\omega_\tau - E_M)I_k/\{(\omega_\tau - E_M)^2 + J^2\sigma_0^2 I_k\}$ and the Fermi distribution function $f(\omega_\tau)$. We find that $K_M^2(\sigma_0^2)$ is an increasing function with respect to σ_0. Therefore, if only the radial (ρ-) fluctuations are effective, the self-consistent order parameter σ_0 is expected to increase from the mean-field solution. On the other hand, σ_0 is expected to decrease for the phase (π-) fluctuations alone, and it is not changed from the mean-field value with both of the fluctuations being into account.

To perform a numerical calculation, we consider the isotropic hybridization ($I_{\vec{k}} = 1$) and half-filled ($N_e = 2$) case with a ratio of J to the conduction band half-width D of $J/D = 1/6$. For this case, we obtain the temperature dependence of the square of the order parameter σ_0^2, which is now proportional to the hybridization gap, as a function of temperature, as shown in figure 2. The solid curve shows σ_0^2 for the 1L radial fluctuations, the dashed curve that for the MFA, and the dash–dotted curve that for the 1L phase fluctuations. Note that the critical index of σ_0^2 is 1 for all the cases. The ratio of the critical temperatures T_c of the 1L radial fluctuations and the MFA is given by $T_c^{(1L)}/T_c^{(MF)} = e^{-6(2\sqrt{6}-5)} \sim 1.83$.

In the 2LA, the first term in the right-hand side of equation (7) is divided into $\Delta F^{(2)}_{FS}$ and $\Delta F^{(2)}_{VS}$, both of which come from the difference of the contraction with respect to that for the bosons. The former consists of the 1L fermion self-energy and the latter the 1L $\{\rho, \pi\}$-fermion vertex corrections, which are given as

$$\Delta F_{FS} = (1/4)k_B T \langle \mathrm{tr}(\hat{M}_f^{k,k+q}\,\hat{G}_0^{k+q}\,\hat{M}_f^{k+q,k}\,\hat{G}_0^k \hat{M}_f^{k,k+q'}\,\hat{G}_0^{k+q'}\,\hat{M}_f^{k+q',k}\,\hat{G}_0^k)\rangle$$

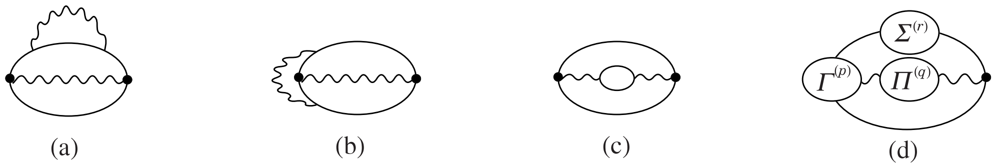

Figure 3. The two-loop diagrams for the free energy $\Delta F^{(2)}$ dressed with: (a) the fermion self-energy, $\Delta F^{(2)}_{\rm FS}$; (b) the fermion–boson vertex corrections, $\Delta F^{(2)}_{\rm VC}$; (c) the boson self-energy $\Delta F^{(2)}_{\rm BS}$. (d) The general structure of the one- and two-loop diagrams, where $\Sigma^{(r)}$, $\Gamma^{(p)}$ and $\Pi^{(q)}$ represent the r-loop fermion self-energy, the p-loop fermion–boson vertex function, and the q-loop boson self-energy, respectively.

and

$$\Delta F_{\rm VS} = (1/4)k_{\rm B}T\langle {\rm tr}(\hat{M}_{\rm f}^{k,k+q}\hat{G}_0^{k+q}\hat{M}_{\rm f}^{k+q,k+q+q'}\hat{G}_0^{k+q+q'}\hat{M}_{\rm f}^{k+q+q',k+q'}\hat{G}_0^{k+q'}\hat{M}_{f}^{k+q',k}\hat{G}_0^{k})\rangle.$$

Here, $\hat{G}_0^k$ and $\hat{M}_{\rm f}^{k+q',k}$ denote four-momentum (momentum and frequency) representations of $\hat{G}_0$ and $\hat{M}_{\rm f}$, respectively. The summations over k, q, and q' must be carried out. The second term in the right-hand side of equation (7) is dressed with the 1L boson self-energy $\Delta F^{(2)}_{\rm BS}$, whose diagram is shown as figure 3(c), and its representation is simply obtained. The one- and two-loop diagrams are regarded as the lowest and the next-lowest ones of figure 3(d). Therefore, it is suggested that the higher-order corrections have the general structure of figure 3(d).

In summary, we have found that in the 1LA the heavy-fermion state is stabilized by radial fluctuations. This is the case if the phase fluctuations are gauge-fixed. One gauge-fixing mechanism may be the Anderson–Higgs mechanism [3, 4], in which the real electromagnetic fields absorb the Nambu–Goldstone mode, although the applicability of this mechanism close to the critical temperature should be examined. We have also obtained the analytical expressions for the two-loop corrections, and numerical calculations based on these are now in progress.

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