Heavy-fermion spin liquid in the strong hybridization limit of the finite-U Anderson lattice model

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Studying the finite-U Anderson lattice model in the strong hybridization limit, we find a heavy-fermion spin liquid phase, where both conduction and localized fermions are strongly hybridized to form heavy fermions but this heavy-fermion phase corresponds to a symmetric Mott insulating state owing to the presence of charge gap, resulting from large Hubbard-U interactions in localized fermions. We show that this heavy-fermion spin liquid phase differs from the "fractionalized" Fermi liquid state, where the latter corresponds to a metallic state with a small Fermi surface of conduction electrons while localized fermions decouple from conduction electrons to form a spin liquid state. We discuss the stability of this anomalous spin liquid phase against antiferromagnetic ordering and gauge fluctuations, in particular, instanton effects associated with confinement of slave particles. Furthermore, we propose a variational wave function to check its existence from the microscopic model.

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I. INTRODUCTION

Spin liquid has been intensively studied, motivated from the resonating-valance-bond (RVB) scenario for anomalous finite temperature physics of the Pseudogap phase in high $T_c$ cuprates.[1] However, such spin liquid physics is fascinating itself because this phase has a nontrivial order called topological or quantum order beyond the description of the Landau-Ginzburg-Wilson paradigm for phase transitions, and its low energy physics is described by a gauge theory, far from the conventional structure of condensed matter theories, allowing spin-fractionalized excitations called spinons.[2]

Recently, several geometrically frustrated insulators are proposed to be genuine symmetric Mott insulating phases, i.e., spin liquids.[3] Although such magnetic frustration can be a strong candidate as the mechanism for the existence of spin liquid, it is still interesting to find another mechanism for its existence. In this paper we propose a heavy-fermion spin liquid phase in the strong hybridization limit of the finite-U Anderson lattice model (ALM).

An important thing is how to suppress magnetic ordering. Antiferromagnetic order is well known to occur at half filling in the square lattice due to Fermi-nesting. One way to suppress the antiferromagnetic ordering is to make spin singlets introducing another band-electrons. Furthermore, if the nesting property can be destroyed, such an ordering tendency will be much more suppressed. This motivates us to consider the ALM since it shows a large Fermi surface when conduction electrons are hybridized with localized electrons.

In this paper we consider the strong hybridization limit, turning on on-site Hubbard interactions to localized electrons. Two possibilities are expected. One is that strong local interactions weaken hybridization, causing the "fractionalized" Fermi liquid phase, where localized fermions form a spin liquid phase while conduction electrons are in the Fermi liquid state.[4] However, Fermi-nesting in the localized fermion-band would result in antiferromagnetic ordering. Magnetically frustrated interactions are required for the fractionalized Fermi liquid to realize. The other is that the hybridization still survives against local interactions, but charge fluctuations are suppressed due to such interactions. Since Fermi-nesting does not exist and Kondo singlets are formed owing to hybridization, antiferromagnetic ordering does not arise, but this corresponds to an insulating state owing to charge gap. Because such a phase contains all symmetries of the original lattice model, it can be identified with a spin liquid state with heavy neutral fermions, i.e., spinons. We propose that this heavy-fermion spin liquid state can emerge in the strong hybridization limit of the finite-U ALM.

To describe Mott transition, it is necessary to take on-site Hubbard interactions non-perturbatively. Recent studies on the Hubbard model have revealed that the slave-rotor representation can treat such interactions well, describing the Mott transition.[5] Applying the U(1) slave-rotor representation to the finite-U ALM, and performing gauge transformation[6] appropriate in the strong hybridization limit, we find an effective U(1) gauge Lagrangian in terms of renormalized conduction and localized fermions and collective density-fluctuation bosons interacting via $U(1)$ slave-rotor gauge fluctuations. We show that such density fluctuations associated with localized fermions become gapped, increasing the Hubbard interaction-U in the strong hybridization limit. This gapped phase is identified with an insulating phase with all symmetries of the ALM, thus heavy-fermion spin liquid. We discuss the stability of the spin liquid phase against gauge fluctuations, in particular, instanton excitations associated with confinement of slave-particles. Furthermore, we propose a variational wave function to check its existence from not the effective field theory but the microscopic model itself.
It should be noted that the heavy-fermion spin liquid phase differs from the fractionalized Fermi liquid state [4] because the former is an insulator, thus there is no Fermi surface while the latter is a metal to have a small Fermi surface of conduction electrons. In this respect the present Mott transition in the ALM should be discriminated from Kondo breakdown as the orbital-selective Mott transition [7]. Furthermore, the spin liquid state in the fractionalized Fermi liquid phase would be unstable against antiferromagnetic ordering owing to the presence of Fermi-nesting.

It is important to notice that the limit considered in this paper is different from that studied in the context of heavy fermion physics [8, 9]. Quantum phase transitions in heavy fermion compounds are studied in the large-U limit of the ALM, where the Kondo lattice model (KLM) or infinite-U ALM is in the main interest. On the other hand, the present study considers the strong hybridization limit, not seriously taken into account in the KLM or infinite-U ALM context.

II. U(1) SLAVE-ROTOR REPRESENTATION OF THE FINITE-U ANDERSON LATTICE MODEL

We start from the finite-U ALM

\[
L_{ALM} = \sum_{i\sigma} c_{i\sigma}^\dagger (\partial_\tau - \mu) c_{i\sigma} - t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.)
- V \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i\sigma} + H.c.) + \sum_{i\sigma} d_{i\sigma}^\dagger (\partial_\tau + \epsilon_d) d_{i\sigma}
+ U \sum_{i} d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow},
\]

where \( c_{i\sigma} \) represents conduction electrons with dispersion \( \epsilon_k^c = -2t(\cos k_x + \cos k_y) \) in two dimensions, and \( d_{i\sigma} \) localized electrons with localized level \( \epsilon_d \).

Quantum phase transitions are expected to occur via competition between the hybridization term with \( V \) and the local interaction term with \( U \). Without the interaction term of \( U \) this model is exactly solvable, resulting in hybridization between the conduction and localized bands. Our problem is to study what happens to the hybridization when the local interaction \( U \) is turned on.

The local interaction term can be decomposed into the charge and spin channels

\[
U \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow} = \frac{U}{4} \sum_i (\sum_{\sigma} d_{i\sigma}^\dagger d_{i\sigma} - 1)^2 - \frac{U}{4} \sum_{\langle ij \rangle} \sum_{\sigma} d_{i\sigma}^\dagger d_{j\sigma} d_{i\sigma} d_{j\sigma} - \frac{U}{2} \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} - \frac{U}{4} \sum_i 1.
\]

In this paper we do not consider the spin channel, justified in the strong hybridization limit where antiferromagnetic ordering is severely suppressed.

Recently, we could describe the genuine Mott transition without symmetry breaking, introducing the slave-rotor representation in order to take into account local interactions non-perturbatively in the Hubbard model [5]. Decomposing the localized electron \( d_{i\sigma} = e^{-i\theta_\sigma} \eta_{i\sigma} \), one can rewrite the ALM in the following way

\[
L_{ALM} = \sum_{i\sigma} c_{i\sigma}^\dagger (\partial_\tau - \mu) c_{i\sigma} - t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.)
- V \sum_{i\sigma} (c_{i\sigma}^\dagger e^{-i\theta_\sigma} \eta_{i\sigma} + H.c.) + \sum_{i\sigma} \eta_{i\sigma} (\partial_\tau + \epsilon_d) \eta_{i\sigma}
+ \frac{U}{4} \sum_i L_i^2 - \frac{U}{2} \sum_i L_i \partial_\tau \theta_i
+ i \sum_{i} \varphi_i (L_i - \sum_{\sigma} \eta_{i\sigma} \eta_{i\sigma} - 1),
\]

where \( \epsilon_d \) is replaced with \( \epsilon_d - U/2 \). It is easy to show that Eq. (3) is exactly the same as Eq. (1) with Eq. (2) after integrating out the \( \varphi_i \) field with \( \eta_{i\sigma} = e^{i\theta_\sigma} d_{i\sigma} \). In this expression the electron Hilbert space \( |d_{i\sigma} \rangle > \) is given by the direct product of the fermion and boson Hilbert spaces \( |\eta_{i\sigma} \rangle > \otimes |L_i \rangle >\) according to the decomposition \( d_{i\sigma} = e^{-i\theta_\sigma} \eta_{i\sigma}, \) where \( L_i \) represents an electron density at site \( i \). It is clear that any decomposition method enlarges the original electron Hilbert space, thus an appropriate constraint associated with the decomposition should be imposed. The Lagrange multiplier field \( \varphi_i \) expresses the U(1) slave-rotor constraint \( L_i = \sum_{\sigma} \eta_{i\sigma} \eta_{i\sigma} - 1 \), implying that the fermion and boson Hilbert spaces are not independent, thus the two operators \( \eta_{i\sigma} \) and \( e^{i\theta_\sigma} \) also. Then, \( e^{-i\theta_\sigma} \) is identified with an annihilation operator of an electron charge owing to the constraint \( L_i = \sum_{\sigma} \eta_{i\sigma} \eta_{i\sigma} - 1 \) and the canonical relation \( [L_i, \theta_j] = -i \delta_{ij} \) imposed by \( -i L_i \partial_\tau \theta_i \). In this respect collective density fluctuations associated with localized fermions can be taken into account non-perturbatively in the U(1) slave-rotor representation.

III. HEAVY FERMION PHYSICS: KONDO BREAKDOWN AS THE ORBITAL-SELECTIVE MOTT TRANSITION

The problem is how to treat the hybridization term with \( e^{-i\theta_\sigma} \). One direct way is to integrate out conduction electrons and obtain an effective Lagrangian in terms of localized fermions and their density-fluctuation bosons [4]. Integrating out the density field \( L_i \) and conduction electron field \( c_{i\sigma} \), we obtain

\[
L_{eff} = \sum_{i\sigma} \eta_{i\tau\sigma} (\partial_\tau + \epsilon_d) \eta_{i\tau\sigma} - i \sum_{ij\tau\sigma} \Delta_{ij\tau\sigma} e^{i\theta_{ij\tau}} \eta_{i\tau\sigma} \eta_{j\tau\sigma} - 1 \]
- \sum_{ij\tau\sigma} \eta_{i\tau\sigma} e^{i\theta_{ij\tau}} \eta_{j\tau\sigma} \eta_{i\tau\sigma} + \frac{1}{U} \sum_i (\partial_\tau \theta_\sigma - \varphi_i)^2.
\]

where \( \Delta_{ij\tau\tau'} \) is the single particle propagator of the conduction electron, given by

\[
\Delta_{ij\tau\tau'}^\epsilon = \frac{V^2}{i\omega + \epsilon_q}.
\]
in the energy-momentum space.

Although the above treatment itself is exact so far, it has an important assumption that the identity of conduction electrons is sustained. In other words, feedback effects of localized fermions and density fluctuations to conduction electrons, self-energy corrections of conduction electrons, are not introduced. Since such feedback effects can be induced only via the hybridization coupling term, this treatment may be regarded as the weak hybridization approach, not justified in the strong hybridization limit.[10] Alternatively, it may be viewed as the large-U-limit approach owing to small \( V/U \) in the hybridization term of Eq. (3). In the small V/U hybridization) limit of the ALM although its mathematical construction is performed at finite-U. In this section we take the strong hybridization approach, considering that the hybridization term is relevant in the renormalization group sense when \( U = 0 \). We show that this type of approach allows a new possible phase called the heavy-fermion spin liquid in the finite-U ALM.

Performing the Hubbard-Stratonovich transformation for the non-local hopping term in both time and space, we obtain an effective Lagrangian

\[
L_{eff} = \sum_{i\sigma} \eta^\dagger_i (\partial_\tau + e_d) \eta_i - i \sum_i \varphi_i (\sum_{\sigma} \eta^\dagger_i \eta_\sigma - 1) \\
+ \sum_q \chi_{q}^{\eta} (\partial_\tau - \mu + e_q^\eta) \chi^\theta_q + \frac{1}{U} \sum_i (\partial_\tau \varphi_i - \varphi_i)^2 \\
- V \sum_{ij} \sum_{\sigma} \eta^\dagger_i \chi^\theta_{ij} \eta_\sigma + \chi^\theta_{ij} \chi_{ij}^\eta e^{-i\theta_j} \tag{5}
\]

where \( \chi_{ij}^{\eta} \) and \( \chi_{ij}^{\theta} \) are effective hopping parameters determined in the self-consistent analysis

\[
\chi_{ij}^{\eta} = V \langle \eta \rangle (\partial_\tau - \mu + e_{ij}^\eta) e^{-i\theta_j}, \\
\chi_{ij}^{\theta} = V \langle \eta \rangle (\partial_\tau - \mu + e_{ij}^\theta) \eta_\sigma). \tag{6}
\]

It is not easy to perform the self-consistent analysis because such effective hopping parameters have both frequency and momentum dependencies (nonlocal in time and space). This non-locality may give rise to crucial effects to the heavy fermion physics. Since this is not our main subject, we leave its detailed analysis in an important future problem, and here, discuss what is expected in this treatment.

Generally speaking, two phases would be allowed in this approximation, determined by the condensation of slave-rotor bosons. In the large V/U limit collective density-fluctuation bosons become condensed, and heavy-fermion Fermi liquid appears to form a large Fermi surface since \( \langle e^{i\theta_i} \rangle \neq 0 \) results in \( \langle e^{i\theta_i} \eta_\sigma \rangle \neq 0 \) as shown in the hybridization term of Eq. (3). In the small V/U limit such boson excitations become gapped, and localized fermions decouple from conduction electrons owing to \( \langle c_{i\sigma} \eta_\sigma \rangle = 0 \), forming a spin liquid state. Such a phase is called the fractionalized Fermi liquid state with a small Fermi surface of conduction electrons.[4] As a result, the heavy-fermion Fermi liquid to fractionalized Fermi liquid transition is identified with Kondo breakdown as the orbital-selective Mott transition[7] in the U(1) slave-rotor representation of the finite-U ALM. However, the spin liquid state would be unstable against antiferromagnetic ordering owing to Fermi-nesting in the square lattice.

Although one important issue, that is, the abrupt volume-change of the Fermi surface at the heavy-fermion quantum critical point,[12] can be explained by the Kondo breakdown transition as discussed above, the fact that the antiferromagnetic transition of localized fermions arises simultaneously at the same quantum critical point as the Kondo breakdown transition is still far from our understanding because such a phenomenon is beyond the description of the Landau-Ginzburg-Wilson theoretical framework for phase transitions.[13] How to incorporate such an antiferromagnetic transition in the Kondo breakdown one is an important open problem.

### IV. STRONG HYBRIDIZATION APPROACH

In the previous section we have discussed the heavy fermion physics in the "large-U" (more accurately, weak hybridization) limit of the ALM although its mathematical construction is performed at finite-U. In this section we take the strong hybridization approach, considering that the hybridization term is relevant in the renormalization group sense when \( U = 0 \). We show that this type of approach allows a new possible phase called the heavy-fermion spin liquid in the finite-U ALM.

#### A. Gauge transformation and effective Lagrangian

The relevance of the hybridization coupling in \( U = 0 \) motivates us to consider the gauge transformation of \( c_{i\sigma} = e^{-i\theta_i} \psi_{i\sigma} \), where this type of approach has been utilized in the context of quantum disordered superconductors[14]. Integrating out the density field \( \varrho_i \) and inserting another slave-rotor decomposition \( c_{i\sigma} = e^{-i\theta_i} \psi_{i\sigma} \) into Eq. (3), we find the following expression

\[
Z = \int D\psi_{i\sigma} D\eta_\sigma D\varphi_i \exp \left\{ - \int d\tau \left\{ \sum_{i\sigma} \psi_{i\sigma} (\partial_\tau - \mu + e_{i\sigma}^\theta) \psi_{i\sigma} + H.c. \right\} \\
- V \sum_{i\sigma} (\psi_{i\sigma}^\dagger \psi_{i\sigma} + H.c.) + \sum_{i\sigma} \eta^\dagger_{i\sigma} (\partial_\tau + e_d) \eta_{i\sigma} \\
- i \sum_i \varphi_i (\sum_{\sigma} \eta^\dagger_{i\sigma} \eta_{i\sigma} - 1) + \frac{1}{U} \sum_i (\partial_\tau \varphi_i - \varphi_i)^2 \right\}. \tag{7}
\]

Couplings between charge fluctuations and renormalized conduction electrons can be decomposed using the Hubbard-Stratonovich transformation. Following Ref.
where the hopping parameters are represented as $\lambda_{ij}$, we find the effective Lagrangian from Eq. (7) 

\[
L_{\text{eff}} = L_0 + L_\psi + L_\eta + L_V + L_\theta,
\]

\[
L_0 = \frac{1}{U} \sum_i q_{ri}^2 - \frac{2}{U} \sum_i q_{ri}(\varphi_{ri} - p_i) + \sum tx y,
\]

\[
L_\psi = \sum_{ij} \psi_\sigma^\dagger(\partial_\tau - \mu)\psi_\sigma - i \sum_q p_i \sum_{\sigma} \psi_\sigma^\dagger \psi_\sigma - 1,
\]

\[
L_\eta = \sum_{ij} \eta_\sigma (\partial_\tau + \epsilon_i^{\text{eff}})\eta_\sigma - i \sum_i (\varphi_{ri} - q_{ri}) \sum_{\sigma} \eta_\sigma^\dagger \eta_{\sigma} - 1,
\]

\[
L_V = -V \sum_{i\sigma} (\psi_\sigma^\dagger \eta_{\sigma} + H.c.),
\]

\[
L_\theta = \frac{1}{U} \sum_i (\partial_\tau \theta_i - \varphi_{ri})^2 - 2t_y \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j + a_{ij}),
\]

where the hopping parameters are represented as $x_{ij} = xe^{i\alpha_{ij}}$ and $y_{ij} = ye^{i\beta_{ij}}$, and $\varphi_i = \varphi_{ri} - q_{ri}$ is used with $q_{ri} = Uq_i/2$. The unidentified parameters can be determined self-consistently in the saddle-point analysis 

\[
p_i = \langle \partial_\tau \theta_i \rangle, \quad q_{ri} = i \frac{U}{2} \sum_{\sigma} \psi_\sigma^\dagger \psi_\sigma - 1,
\]

\[
x = |\langle e^{-i\theta_j} e^{i\theta_j} + H.c. \rangle|, \quad y = |\langle \sum_{\sigma} \psi_\sigma^\dagger \psi_{\sigma} + H.c. \rangle|.
\]

(9)

$p_i$ and $q_{ri}$ play the role of renormalization for the fermion and boson chemical potentials, respectively.

The effective Lagrangian Eq. (8) is the main result of this paper, showing an important feature of the finite-U ALM, that is, the presence of two kinds of relevant interactions. As mentioned before, the hybridization coupling is relevant to give rise to a band-hybridized metal if the local charge-fluctuation energy is not taken into account. On the other hand, an appropriate treatment of local charge fluctuations has been shown to result in the Mott transition from a spin liquid to a Fermi liquid at a critical value $U_c$ without hybridization, i.e., in the Hubbard model.[5]

Compared to the effective Lagrangian Eq. (5) for the heavy-fermion quantum phase transition, the effective Lagrangian Eq. (8) always allows the band-hybridization while Eq. (5) does not. In Eq. (5) the boson condensation corresponds to the hybridization transition since it gives an effective hybridization coupling constant $V_{\text{eff}} = |\langle e^{i\theta_j} \rangle|V$. Such a transition is involved with the abrupt volume change of the Fermi surface. On the other hand, in Eq. (8) the renormalized conduction and localized fermions are always hybridized, forming a large Fermi surface of spinons (neutral fermions). Then, the boson condensation in Eq. (8) corresponds to the genuine Mott transition in these heavy fermions.

Since the slave-rotor variable has its own dynamics in the saddle-point approximation, given by the U(1) rotor (XY) model, the quantum transition described by condensation of the rotor field occurs when $D_y/U \sim 1$ with the half bandwidth $D$, where $D_y$ is an effective bandwidth for the rotor variable.[15] It is important to understand that the ratio $V/U$ between the hybridization and on-site interactions controls the hopping parameter $y$, where the hopping parameter decreases as this ratio decreases. This results in the quantum critical point $(V/U)_c$ between the heavy-fermion Fermi liquid and heavy-fermion spin liquid, which differs from the heavy-fermion quantum critical point between the heavy-fermion and fractionalized Fermi liquids.

It is interesting to notice that this treatment [Eq. (8)] gives rise to two different energy scales.[16] One corresponds to the bandwidth/hybridization scale $T_K$, and the other is associated with the coherence scale $T_{FLK}$, resulting in a Fermi liquid. $T_K$ is proportional to the hybridization gap $V$ in the strong coupling approach, consistent with the single impurity energy scale in the strong coupling limit. On the other hand, $T_{FLK}$ is proportional to the effective stiffness parameter $D_y|\langle e^{i\theta_j} \rangle|^2$ controlling the coherence of $\theta_i$.[17]

### B. Mean-field analysis

For the saddle-point analysis we resort to large $N$ generalization replacing $e^{i\theta_j}$ with $\phi_{ks}$, where $s = 1, \ldots, N$.[18] Taking the mean-field ansatz of $i\rho_i = p$, $i\varphi_{ri} = \varphi_r$, $iq_{ri} = -q_r$, and $i\lambda_i = \lambda$ where $\lambda$ introduces the rotor constraint $\sum_s |\phi_{ks}|^2 = 1$, we obtain the free energy functional

\[
F_{MF} =
\]

\[
-\frac{1}{\beta} \sum_{k\sigma} \sum_{\omega_n} \ln(i\omega_n - E_{k^+}) - \frac{1}{\beta} \sum_{k\sigma} \sum_{\omega_n} \ln(i\omega_n - E_{k^-})
\]

\[
+ \frac{1}{\beta} \sum_{k} \sum_{\nu_n} \ln\left(-\frac{1}{U} [i\nu_n + \varphi_r]^2 + ye^\phi + \lambda \right)
\]

\[
+ \sum_k \left(Dxy - \frac{2}{U} q_r [p + \frac{q_r}{2}] + p + \varphi_r + q_r \right)
\]

\[
- \lambda + \mu[1 - \delta].
\]

(10)

Here the renormalized fermion spectrum is given by $E_{k \pm} = \frac{[(\omega_n + \mu - p) + (\omega_n - \varphi_r)]}{2} \pm \sqrt{[(\omega_n + \mu - p) - (\omega_n - \varphi_r)]^2 + V^2}$, and $\delta$ is hole concentration for the conduction band. $\omega_n (\nu_n)$ is the Matzubara frequency for fermions (bosons).

Minimizing the free energy Eq. (10) with respect to $\lambda$, $x$, $y$, $q_r$, $\varphi_r$, $p$, and $\mu$, we obtain the self-consistent mean-field equations. Performing the Matzubara frequency summations and momentum integrals with $\sum_k =
\[
\frac{1}{2D} \int_{-D}^{D} d\epsilon \text{ (constant density of states[5, 18]), we find }
\[
1 = \sqrt{U(\lambda + Dy)} - \sqrt{U(\lambda + y\epsilon_0)} = \frac{1}{\epsilon_0} \left( \frac{\epsilon_0^2 + \lambda}{U} - \lambda \right),
\]
\[
x = \frac{(2\lambda - Dy)\sqrt{U(\lambda + Dy)} - (2\lambda - y\epsilon_0)\sqrt{U(\lambda + y\epsilon_0)}}{3(Dy)^2},
\]
\[
y = \frac{1}{3} \left( 1 - \frac{\epsilon_0^2}{D^2} \right) + \frac{V^2}{2D^2} \left[ \ln \left( \frac{\sin[\tan^{-1}(\frac{\epsilon_0 - \mu_c}{2V})] - \frac{1}{\epsilon_0}}{-\sin[\tan^{-1}(\frac{\epsilon_0 - \mu_c}{2V})] + \frac{1}{\epsilon_0}} \right) \right. \\
- \ln \left( \frac{\sin[\tan^{-1}(\frac{\epsilon_0 - \mu_c}{2V})] + \frac{1}{\epsilon_0}}{-\sin[\tan^{-1}(\frac{\epsilon_0 - \mu_c}{2V})] + \frac{1}{\epsilon_0}} \right) \\
- \left. \frac{1}{\epsilon_0} \right] \left( 1 - \frac{\epsilon_0^2}{D^2} \right) + \frac{V^2}{2D^2} \left[ \ln \left( \frac{\cos[\tan^{-1}(\frac{\epsilon_0 - \mu_c}{2V})] + \frac{1}{\epsilon_0}}{-\cos[\tan^{-1}(\frac{\epsilon_0 - \mu_c}{2V})] + \frac{1}{\epsilon_0}} \right) \right. \\
+ \frac{1}{\epsilon_0} \right] \left( 1 - \frac{\epsilon_0^2}{D^2} \right) + \frac{V^2}{2D^2} \left[ \tan^{-1}(\frac{\epsilon_0 - \mu_c}{2V}) \right] \\
- \frac{1}{\epsilon_0} \right]
\]
\[
\epsilon_\psi = \frac{1}{x} \left( \frac{\epsilon_d - q_r - \varphi_r}{\epsilon_d + \epsilon_\psi + \mu + p} \right),
\]
\[
\frac{2}{U} (\varphi_r - p + q_r) - 1 = \frac{1}{2} \left( 1 + \frac{\epsilon_\psi}{D} \right)
\]
\[
- \frac{V}{D\epsilon_\psi} \left[ \ln \left( \frac{\cos[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] + \frac{1}{\epsilon_\psi}}{-\cos[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] + \frac{1}{\epsilon_\psi}} \right) \right. \\
\left. + \frac{1}{\epsilon_\psi} \right] \left( 1 - \frac{\epsilon_\psi^2}{D^2} \right) + \frac{V}{D\epsilon_\psi} \left[ \tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V}) \right]
\]
\[
\frac{2}{U} (\varphi_r - p) = \left( 1 + \frac{\epsilon_\psi}{D} \right) = \left( 1 - \frac{\epsilon_\psi}{D} \right), \quad q_r = -\frac{U}{2} \delta, \quad \mu_r = \mu + p + \epsilon_d - q_r - \varphi_r.
\]
\]
\[
\frac{2U}{D} = \frac{V^2}{2(D/3)^2} \left[ \ln \left( \frac{\sin[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] - \frac{1}{\epsilon_\psi}}{-\sin[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] + \frac{1}{\epsilon_\psi}} \right) \right. \\
- \ln \left( \frac{\sin[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] + \frac{1}{\epsilon_\psi}}{-\sin[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] + \frac{1}{\epsilon_\psi}} \right) \\
- \left( \frac{1}{\epsilon_\psi} \right) \left( 1 - \frac{\epsilon_\psi^2}{D^2} \right) + \frac{V^2}{2D^2} \left[ \ln \left( \frac{\cos[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] + \frac{1}{\epsilon_\psi}}{-\cos[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] + \frac{1}{\epsilon_\psi}} \right) \right. \\
+ \frac{1}{\epsilon_\psi} \right] \left( 1 - \frac{\epsilon_\psi^2}{D^2} \right) + \frac{V^2}{2D^2} \left[ \tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V}) \right]
\]
\[
\delta = \frac{V}{D/3} \left[ \cos[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] - \cos[\tan^{-1}(\frac{\epsilon_\psi - \mu_c}{2V})] \right], \quad \mu_r = \frac{D}{3} - \left( \frac{V^2}{\epsilon_d + U\delta} - \frac{\epsilon_d + U/2\delta}{\epsilon_\psi} \right).
\]

Actually, we find (0.112, 0.044) at \( \delta = 0.800 \) and \( \epsilon_d/D = -0.001 \), thus \( (V/U)_c = 2.545 \).

This quantum phase transition results from gapping of density fluctuations of localized fermions in the presence of strong hybridization with renormalized conduction fermions, thus differing from the Kondo breakdown transition[4] in the ALM. In \( V/U > (V/U)_c \) collective density fluctuations become softened, and the saddle-point equation of \( \lambda \) is replaced with \( 1 = \sqrt{2U/Dy} + Z \), where \( Z = |\langle \epsilon_\psi^0 \rangle|^2 \) is the condensation amplitude. Thus, the coherence temperature is given by \( T_{FL} \approx (Dy - 2U)^{1/2} \) near the heavy-fermion Mott critical point, and below this temperature the valence-fluctuation-induced heavy-fermion phase arises.

V. HEAVY-FERMION SPIN LIQUID TO HEAVY-FERMION FERMI LIQUID QUANTUM TRANSITION: ITS CRITICAL FIELD THEORY AND NON-FERMI LIQUID PHYSICS

To investigate low energy physics near the heavy-fermion spin liquid to Fermi liquid quantum critical point, we derive an effective field theory from Eq. (8). From the mean-field Lagrangian
\[
L_\chi = \sum_{k\sigma} \chi_{k\sigma} (\psi_{k\sigma} + \psi_{k\sigma}^\dagger) + \sum_{k\sigma} (\mu_c - \epsilon_k) \chi_{-k\sigma} - \sum_{k\sigma} (\mu_c - \epsilon_k)
\]
where \( \psi_{k\sigma} = u_k \chi_{k\sigma}^+ + v_k \chi_{k\sigma}^- \) and \( \mu_c = v_k \chi_{k\sigma} + u_k \chi_{k\sigma}^- \) with \( u_k = V/\sqrt{(E_k^+ - \epsilon_k)^2 + V^2} \) and \( v_k = -(E_k^+ - \epsilon_k)^2 + V^2 \), we find its critical field theory \( L_\chi = \chi_{-k\sigma} (\psi_k - \mu_c) \chi_{-k\sigma}^+ + \frac{1}{2} \chi_{-k\sigma} \chi_{-k\sigma} \). Here the renormalized fermion field \( \chi_{-k\sigma} \) represents \( \chi_{-k\sigma} \) in the continuum limit, and the effective band mass is given by \( m_\chi = \left( \partial^2 E_k^- / \partial k^2 \right)^{-1} = m_c / \left[ \frac{4\epsilon_d}{\epsilon_d + V^2} - 1 \right] \) with the "bare" band mass
$m_\phi \sim (lx)^{-1}$, renormalized localized level $\epsilon_{dr} = \epsilon_d + \frac{U}{2} \delta$, and critical chemical potential $\mu_c$. Note that $m_\chi$ diverges in the limit of $V \to \infty$.

The effective boson Lagrangian can be written with an electromagnetic field $A$ as $\mathcal{L}_b = [(\partial_\mu - i \varphi_\mu)] [(\partial_\mu - i \varphi_\mu) \phi_{rs}^2] + |(\nabla - i a_r - i A) \phi_{rs}|^2 + m_\phi^2 |\phi_{rs}|^2 + \frac{1}{2} |\phi_{rs}|^4$, where the rotor field $e^{i \theta_r}$ is replaced with $\phi_{rs}$, and the rotor constraint is softened via introduction of local interactions $u_\phi$. $m_\phi$ is an effective mass, given by $m_\phi^2 = (V/U) \epsilon_c - (V/U)$. An important point is that the renormalized boson chemical potential $\varphi_\mu$ becomes zero at the quantum critical point ($m_\phi^2 = 0$), thus the linear time-derivative term vanishes.

We find the critical field theory at the heavy-fermion spin liquid quantum critical point

$$S_c = \int d^d x \left( \frac{1}{2m_\chi} |(\nabla - i a_r) \chi_{rs}|^2 + |(\nabla - i a_r - i A) \phi_{rs}|^2 + \frac{1}{2} |\phi_{rs}|^2 \right) + S_{eff}[a_r],$$

where the critical gauge action is given by $S_{eff}[a_r] = \frac{1}{2} \sum_{q,\omega} \left( \gamma_F \frac{\omega}{q} + \frac{N}{2\pi} q \right) (\delta_{ij} - \frac{2q_i q_j}{q^2}) a_{ir} a_{jr}$ with the damping strength $\gamma_F = k_F/\pi$ and boson flavor number $N$.[18] The first term represents dissipative dynamics in gauge fluctuations due to particle-hole excitations of $\chi_{rs}$ fermions near the Fermi surface, and the second term arises from critical boson fluctuations at the quantum critical point.[18] The Maxwell gauge action is omitted since it is irrelevant in the renormalization group sense. Note that the time component of the gauge field mediates a local interaction, thus safely ignored in the low energy limit.[19]

In the random phase approximation one finds the following expression for the free energy $F/V = \int \frac{d^d q}{(2\pi)^d} \int \frac{\omega}{2\pi} \coth \left( \frac{\omega}{2T} \right) \tan^{-1} \left[ \frac{\text{Im} D(q,\omega)}{\text{Re} D(q,\omega)} \right]$, where the gauge kernel is given by $D(q,\omega) = \left( -i \gamma_F \frac{\omega}{q} + N \frac{\omega}{2\pi} q \right)^{-1}$ in real frequency at the quantum critical point. This free energy leads to the divergent specific heat coefficient $\gamma = C_V/T \propto -\ln T$. The dc conductivity is given by the Ioffe-Larkin combination-rule $\sigma_{tot} = \sigma_\phi \sigma_\chi / (\sigma_\phi + \sigma_\chi)$, assuming gaussian gauge fluctuations.[20] In the one loop diagram of gauge-boson exchange one finds $1/\tau_\chi \sim T^2$[18] and $1/\tau_\phi^2 \sim T^4$[19], where $1/\tau_\chi$ ($1/\tau_\phi^2$) is the scattering rate of the $\chi_{rs}$ fermion ($\phi_{rs}$ boson) with temperature $T$. As a result, the total dc conductivity is given by $\sigma_{tot} \sim T^{-1}$ in low temperatures, giving rise to the linear resistivity $\rho_{tot} \sim T$ at the quantum critical point. On the other hand, in $V/U < (V/U)_c$ but $|V/U - (V/U)_c| \to 0$ corresponding to the heavy-fermion spin liquid state in the zero temperature limit, the gauge kernel shows the crossover behavior from $D(q,\omega) = \left( -i \gamma_F \frac{\omega}{q} + N \frac{\omega}{2\pi} q \right)^{-1}$ to $D(q,\omega) = \left( -i \gamma_F \frac{\omega}{q} + \frac{\omega}{2\pi} q \right)^{-1}$ with an effective internal gauge-charge $g$ as temperature goes down. Here the crossover energy scale would be an excitation gap of $\delta_{rs}$, given by $|\varphi_\mu|$. Accordingly, the specific heat coefficient exhibits the upturn behavior from $\gamma \sim -\ln T$ to $\gamma \sim T^{-1/3}$. But, the resistivity still behaves as $\rho_{tot} \sim T$ owing to $\rho_{tot} \sim T^{4/3}$ in the $z = 3$ critical field theory.[19] where $z$ is the dynamical exponent.

VI. DISCUSSION AND SUMMARY

A. Stability of the heavy-fermion spin liquid against gauge fluctuations

The stability of the heavy-fermion spin liquid state against gauge fluctuations is an important problem for this phase to realize in the finite-U ALM. It has been shown that the fermion-gauge action in Eq. (13), obtained via integrating out gapped boson excitations, has an infrared stable interacting fixed point with an effective nonzero internal charge when the flavor number or density of fermions is sufficiently large.[21] Actually, the present author has studied that such a fixed point can arise when the fermion conductivity, given by its current-current correlation function, is sufficiently large.[22] Notice that the fermion conductivity is associated with the density of fermions. At this fixed point the critical field theory is characterized by the dynamical exponent $z = 3$, as discussed before.

The problem is the stability of this fixed point against instanton excitations resulting from compact gauge fluctuations. A similar situation appears in the compact QED$_3$, where Dirac fermions interact via compact U(1) gauge fluctuations. The infrared interacting fixed point in the QED$_3$ has been shown to be stable against instanton fluctuations since the scaling dimension of an instanton insertion operator is proportional to the flavor number of massless Dirac fermions, thus irrelevant in the large flavor limit.[23] Following the similar strategy with this case, the present author has shown that the scaling dimension of the instanton operator is proportional to the fermion conductivity analogous to the flavor number of Dirac fermions, thus irrelevant in the large conductivity limit.[22] This seems to be natural because the fermion conductivity is associated with screening of gauge interactions.

In the heavy-fermion spin liquid phase the fermion conductivity may not be sufficiently large because the strong hybridization makes the hybridized band flat. Intuitively, the existence of the heavy-fermion spin liquid phase is not clear because the strong hybridization coupling is necessary for its existence, but such hybridization prohibits this phase from being stable against gauge fluctuations. Since its stability depends on the fermion conductivity, [22, 24] to determine its presence with gauge interactions is beyond the scope of the present study. However, its existence is allowed in principle.

The stability of this phase against antiferromagnetic ordering is confirmed since the Fermi-surface nesting does
not exist in the heavy-fermion band. This not only justifies our neglect of spin fluctuations, but also propose new mechanism for the existence of the spin liquid phase.

B. A variational wave function

The above discussion motivates us to find the heavy-fermion spin liquid phase from the microscopic model itself, here the finite-U ALM. In this respect we propose a variational wave function for its existence. Since we start from the conduction-valance hybridized state, the following wave function is naturally proposed

\[ \left| \Phi \right> = \Pi_{k} (c_{k \sigma}^\dagger + a(k)d_{k \sigma}^\dagger) |0\rangle, \]

where \( |0\rangle \) is the vacuum state and \( a(k) \) is the variational parameter defined by

\[ a(k) = V/[\epsilon_{k}^\dagger - \mu - \epsilon_d]/2 + \sqrt{[\epsilon_{k}^\dagger - \mu - \epsilon_d]^{2}/4 + V^2} \]

in \( U = 0 \). Turning on on-site interactions to localized electrons, the variational ground state is proposed to be

\[ |\Psi\rangle = P_{PG}|\Phi\rangle \]

\[ = \Pi_{i}(1 - \kappa n_{i}^{d} n_{i}^{\dagger}) \Pi_{k} (c_{k \sigma}^\dagger + a(k)d_{k \sigma}^\dagger)|0\rangle \]

where \( P_{PG} = \Pi_{i}(1 - \kappa n_{i}^{d} n_{i}^{\dagger}) \) is the partial Gutzwiller projector, suppressing charge-fluctuation effects, with an interaction-dependent \( \kappa \) determined self-consistently as a function of \( U \).[26]

Since this ground-state wave function captures both relevant interactions, \( V \) and \( U \) appropriately, physics included in Eq. (15) is expected to be essentially imposed in the slave-rotor effective gauge theory [Eq. (8)]. When gauge fluctuations are ignored as the saddle-point approximation in Eq. (8), the \( |\Phi\rangle \) state is exactly recovered from the fermion Lagrangian \( L_{F} = L_{\psi} + L_{\eta} + L_{V} \) because \( L_{F} \) gives rise to the same \( a(k) \) in \( |\Phi\rangle \). Note that the gauge transformation \( c_{\sigma} = e^{-i\theta} \psi_{\sigma} \) is an essential procedure for obtaining this strong hybridized dynamics. On the other hand, the partial Gutzwiller projection operator \( P_{PG} \) is simulated in the slave-rotor representation, \( L_{\theta} \) taking into account on-site interactions of localized electrons appropriately. This approach is parallel to that in the doped Mott insulator problem, where the Gutzwiller projected BCS wave function, i.e., the RVB state had been proposed,[27] and such a variational ground state was simulated in the context of the gauge theory.[1] It will be an interesting project to check whether this ground state wave function can result in both the fractionalized Fermi liquid and heavy-fermion spin liquid.

C. Summary

In this paper we have studied the finite-U ALM in the strong hybridization limit. The conventional treatment, integrating out conduction electrons to obtain an effective Lagrangian in terms of localized fermions and collective density-fluctuation bosons, describes the heavy-fermion quantum transition from the heavy-fermion Fermi liquid with a large Fermi surface to the fractionalized Fermi liquid with a small Fermi surface, where the abrupt volume change of the Fermi surface is involved. On the other hand, the strong hybridization approach shows the heavy-fermion spin liquid to heavy-fermion Fermi liquid transition, where this type of Mott transition differs from the orbital-selective one via Kondo breakdown.

We propose a schematic phase diagram of the finite-U ALM in Fig. 1, where HF-FL, HF-SL, and F-SL represent the heavy-fermion Fermi liquid, heavy-fermion spin liquid, and fractionalized Fermi liquid, respectively. It is important to notice that this model has two independent parameters scaled by the conduction bandwidth, \( (V/D, U/D) \). In the small \( U/D \) limit the hybridization coupling is relevant to form a hybridized band, thus the heavy-fermion Fermi liquid arises. In the large \( U/D \) limit the Kondo breakdown transition has been shown to occur in the KLM or infinite-U ALM, thus there is a critical \( V/D \) separating the fractionalized Fermi liquid \( \langle c_{\sigma}^{\dagger} \eta_{\sigma} \rangle = 0 \) from the heavy-fermion Fermi liquid \( \langle c_{\sigma}^{\dagger} \eta_{\sigma} \rangle \neq 0 \). On the other hand, in the large \( V/D \) limit the heavy-fermion band is formed first \( \langle e^{-i\theta} \rangle = 0 \rightarrow \langle c_{\sigma}^{\dagger} \eta_{\sigma} \rangle \approx (e^{-i\theta}) \langle e^{-i\theta} \rangle \psi_{\sigma}^{\dagger} \eta_{\sigma} = 0 \rangle \) in this heavy-fermion band.

We proposed the variational ground-state wave function for the finite-U ALM since the stability of the heavy-fermion spin liquid state against compact gauge fluctuations cannot be fully confirmed in the effective field theory approach, thus it is necessary to check its existence from the microscopic model. It will be interesting to observe such a spin liquid state in the strong hybridization and large repulsion limits, where the heavy-fermion band still exists, but this corresponds to an insulator owing to charge gap.

We close this paper discussing the possibility of
valence-fluctuation-induced superconductivity.[28] Recently, we have generalized the U(1) slave-rotor formulation of the Hubbard model into the SU(2) one, allowing not only local density fluctuations but also pairing excitations.[5] Both collective charge fluctuations form an SU(2) slave-rotor matrix field, where its off-diagonal components are associated with superconductivity. We believe that the SU(2) slave-rotor decomposition is also available to the finite-U ALM. This superconducting mechanism may explain physics in $PuCoGa_5$, where superconductivity occurs with HF physics at the same time.[9, 29] This interesting possibility is under investigation.

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[10] A similar situation also happens in the magnetic transition of itinerant electrons, described by the Hertz-Moriya-Millis theory [T. Moriya and J. Kawabata, J. Phys. Soc. Jpn. 34, 639 (1973); T. Moriya and J. Kawabata, J. Phys. Soc. Jpn. 35, 669 (1973); J. A. Hertz, Phys. Rev. B 14, 1165 (1976); A. J. Millis, Phys. Rev. B 48, 7183 (1993)]. Since feedback effects to the electron degrees of freedom by order parameter fluctuations are not taken into account, this Landau-Ginzburg-Wilson-type approach should be regarded as a weak coupling one, not justified in the strong coupling limit.[18]
[11] In the single impurity Anderson model Florens and Georges integrate out conduction electrons, and obtain an effective Lagrangian in terms of localized spinons $\eta_\sigma$ and holons $e^{i\phi}$ at the impurity site using the Hubbard-Stratonovich transformation [S. Florens and A. Georges, Phys. Rev. B 66, 165111 (2002)]. They derive self-consistent equations for spinon and holon self-energies, which coincide with the non-crossing approximation framework of the slave-boson theory.
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[13] One cautious person may claim that the slave-particle framework is not appropriate for the Landau-Ginzburg-Wilson forbidden quantum transition in the heavy-fermion context since no local gauge-invariant Kondo order parameter exists, and no symmetry is broken in the Fermi-liquid ground state while the Fermi liquid description in the slave-particle context is in the condensation of slave-bosons, thus breaking the internal U(1) gauge symmetry inevitably. This statement is only partially correct. This situation reminds us of the characterization of superconductivity. Usually, we interpret superconductivity as the condensed phase of Higgs bosons (Cooper pairs). This identification necessarily breaks the U(1) gauge symmetry, thus cannot be correct in a rigorous manner. However, we should admit that this characterization is useful. The way to understand this identification is to break the gauge symmetry explicitly, fixing one gauge. Since the gauge symmetry is explicitly broken via gauge fixing, one can define the local order parameter such as Cooper pair bosons. This is a physically appealing way to understand such a boson-condensed phase in a simple mean-field manner.
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[15] Consider the boson-Hubbard model $H = -t \sum_{\langle ij \rangle} (\bar{b}_i \bar{b}_j + H.c.) + \frac{U}{2} \sum_i n_i^{\sigma} n_i^{\bar{\sigma}}$ with $n_i = \bar{b}_i^\dagger b_i$. Using $b_i = \sqrt{n} e^{i\phi_i}$.
and integrating out the $n$ field, one can obtain the Lagrangian of this Hamiltonian, $L = \frac{1}{2n} \sum (\partial_t \theta_i)^2 - 2tn \sum \cos(\theta_i - \theta_j)$, the same as $L_0$ of Eq. (8) in the mean-field approximation. It is clear that this boson Hubbard model shows the QPT from the Mott insulating phase to the superfluid state at $D/U \sim 1$.

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[17] One need not be surprised at $T_K \sim V$ (instead of the exponentially small $T_K$) in the strong hybridization limit because this is a usual result of the mean-field treatment, considering the antiferromagnetic case (Hartree-Fock calculation) where the magnetization order parameter is exponentially small in the small-U limit of the Hubbard model while it is proportional to Hubbard-U in the large-U limit. In the strong hybridization approach the coherence temperature $T_{FL}$ would be exponentially small, corresponding to the boson-condensation temperature. On the other hand, in the conventional heavy-fermion metal-to-metal transition discussed in section III, the Kondo temperature $T_K$ will be exponentially small since this corresponds to the weak hybridization approach, where $V_{eff} = |\langle e^{-i\theta}\rangle| V$ is an effective hybridization coupling constant with the boson-condensation amplitude $|\langle e^{-i\theta}\rangle|$. Actually, in the single-impurity Anderson model this was indeed found in the non-crossing approximation scheme.[11]

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$$Z \approx \int D\psi D\eta D\theta D\alpha \exp \left[ - \left( \frac{\delta^2 S_\psi}{\delta \alpha} + \frac{\delta S_\psi}{\delta A} \right) a - \frac{1}{2} \frac{\delta^2 S_\eta}{\delta \alpha} \alpha^2 \right]$$

$$- \frac{1}{2} \left( \frac{\delta^2 S_\eta}{\delta \alpha} + \frac{\delta S_\eta}{\delta A} \right) a^2 + 2 \frac{\delta^2 S_\eta}{\delta \alpha \delta A} a A + \frac{\delta^2 S_\eta}{\delta A^2} A^2$$

$$= Z_0 \exp \left[ - \frac{1}{2} \frac{\delta^2 S_\psi}{\delta \alpha^2} \alpha^2 \right]$$

$$+ \frac{1}{2} \left( \frac{\delta^2 S_\eta}{\delta \alpha \delta A} \right)^2 A^2$$

with $Z_0 = \int D\psi D\eta D\theta e^{-\left( S_\psi(0) + S_\eta(0) + S_\alpha(0) \right)}$, where the super- or sub-script $(0)$ means $a = 0$ in the saddle-point approximation. Differentiating the above effective action by an electromagnetic field $A_t$ twice, one can obtain the Ioffe-Larkin conductivity expression, $\sigma_{tot} = \sigma_\theta \sigma_\psi / (\sigma_\theta + \sigma_\psi)$, where $\sigma_\theta = \frac{\delta^2 S_\psi}{\delta \alpha \delta A} |_{\alpha = 0}$, $\sigma_\psi = \frac{\delta^2 S_\eta}{\delta A^2} |_{A = 0}$ and $\sigma_\psi = \frac{\delta^2 S_\psi}{\delta \alpha^2} |_{\alpha = 0}$ Here, the saddle-point condition

$$\left( \frac{\delta S_\psi}{\delta \alpha} \right)_{\alpha = 0} + \left( \frac{\delta S_\eta}{\delta \alpha} \right)_{\alpha = 0} \equiv \langle J_\psi + J_\eta \rangle = 0$$

is imposed in the Ioffe-Larkin formulation.

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