Critical spin liquid phase in the presence of Kondo frustration

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The heavy fermion phase is expected to be robust in the periodic Anderson lattice systems when the density of states of conduction electrons at the Fermi energy is finite. In such systems the spin liquid phase driven by geometrical frustration usually coexist with Kondo screening. Here we study a periodic Anderson-Heisenberg triangular lattice model with both geometric and Kondo frustrations, the latter being caused by the on-site and the nearest neighbor site c-f hybridizations. We show the existence of the Kondo breakdown quantum phase transition at a critical hybridization strength V_c below which the dynamically-decoupled local moment spin liquid phase emerges. Such phase is closely linked to the nodal points of the hybridization function in the presence of Kondo frustration.

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I. INTRODUCTION

Heavy fermion behaviors and the associated quantum magnetism in correlated electron materials have attracted intensive research interests in the society of condensed matter physics [1,2]. The heavy fermion state in these materials develops at low temperatures due to the quantum coherence of Kondo effect, the latter being driven by the Kondo coupling or the orbital hybridization between itinerant and local or f electrons [3–5]. The strong correlation effect comes from the Coulomb repulsion between f electrons, which is expected to be strong enough leading to the localization of f electrons in the absence of hybridization. With the finite hybridization, Kondo effect takes place and is influenced by various spin-spin exchange interactions between local electrons [6,7], which could be mediated either by the Kondo coupling, the so-called Ruderman-Kittel-Kasuya-Yosida interaction [8], or by adjacent ions in realistic materials environments [9–11]. Usually, the interplay of Kondo effect and RKKY interaction is expected to result in the paramagnetic heavy fermion state and the magnetically ordered state, and the competition between them can be captured by the Doniach phase diagram [12].

Interestingly, there is growing evidence of rich quantum phases that are beyond the description of the Doniach scenario [13,14]. For instance, the measurements of Yb-based heavy fermion materials have revealed the existence of the non-Fermi liquid (NFL) state in a finite region of their quantum phase diagrams [2,15–17]. Furthermore, the transport and susceptibility measurements of Ge-substituted $YbRh_2Si_2$ indicate the existence of the quantum spin liquid state exhibiting the NFL features and separating the antiferromagnetic ordered and the paramagnetic Landau fermion liquid states [18]. Another class of material's candidate hosting both Kondo heavy fermion metal and quantum spin liquid state is the transition-metal dichalcogenide bilayers [19–21]. All these point to the important role played by the local spin quantum fluctuations or the quantum zero-point motions enhanced by the geometric frustration in given lattice configurations [14,18,22–25].

The existence of the geometrically frustrated spin liquid state in heavy fermion systems has been theoretically proposed for years [23,26–30]. The stability of the spin liquid state owing to the Kondo screening which reduces the size of local moments was first proposed in Ref. [26]. Recently, the Z_2 metallic spin liquid state is proposed in the $Sp(N)$ extension of the Kondo-Heisenberg model on frustrated lattice with a large N, while the decrease of N will lead to the antiferromagnetically ordered phase [30]. Despite these advances, the existence of the spin liquid phase closed to the boundary of the local moment regime in the heavy fermion systems (with $N = 2$) still needs to be explored.

As a platform of rich spin liquid states, the spin 1/2 antiferromagnet consisting of purely localized electrons on triangular lattices is known as a prototype frustrated spin system [31]. Although its ground state owns the 120° Néel order with reduced magnetic moments [32,33], the fragile magnetic order is expected to break down when compassed by competing quantum effects, leading to the quantum spin liquid phase [34–37]. In realistic f electron compounds, however, it is also possible that the local spin moments are completely screened by conduction electrons leading to the destruction of the spin liquid state. Specifically, as in the canonical periodic Anderson model on the triangular lattice, the density of the state of conduction electrons at the Fermi energy is always finite, a nonzero hybridization strength V will lead to the heavy fermion phase accompanied with a large Fermi surface contributed by both conduction and f electrons. To seek a possible finite hybridization strength V_c below which there is a dynamically decoupled local spin liquid phase accompanied with a small Fermi surface contributed sorely by the conduction electrons, the authors of Ref. [29] proposed a mechanism driven by the kinetic energy of the correlated electrons in a more general Anderson-Hubbard model with a tunable on-site Coulomb repulsion U.

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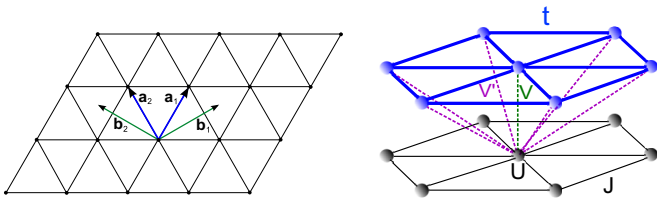

FIG. 1. (a) The triangular lattice. $\mathbf{a}_1$ and $\mathbf{a}_2$ are the lattice basis vectors and $\mathbf{b}_1$ and $\mathbf{b}_2$ are the reciprocal lattice vectors. (b) The diagrammatic sketch for the interactions. The conduction and the correlated (or local) electrons are drawn in the upper and bottom layers, respectively.

In the present work, we propose an alternative route to the existence of the critical hybridization for such spin liquid phase in the local moment regime of correlated electron systems. For this purpose we study a variant of the periodic Anderson triangle lattice model with the antiferromagnetic RKKY interaction as well as with the Kondo screening effect, the latter is driven by both the on-site and the nearest neighbor site Kondo hybridizations. In general, such local and nonlocal hybridizations coexist in realistic correlated electron materials. While they can lead to the usual Kondo screening effect cooperatively in the large U regime, their coexistence may give rise to an intrinsic Kondo frustration, destabilizing the antiferromagnetic ordering of the local moments. In particular, the Kondo frustration leads to the destructive interference characterized by the nodal points of the hybridization function in the momentum space. By tuning the electron filling, the system's band structure is reconstructed at a critical hybridization below which the spin liquid state with a spinon Fermi surface decouples from the conduction electrons due to a delicate destruction of the Kondo screening. In the following, we shall illustrate how this scenario takes place in the corresponding Anderson triangular lattice model by using the slave rotor technique and perturbation theory.

II. MODEL HAMILTONIAN

The configuration of the triangular lattice is illustrated in Fig. 1. The lattice constant is set to unit. The basis vectors are $\mathbf{a}_1 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$ and $\mathbf{a}_2 = (-\frac{1}{2}, \frac{\sqrt{3}}{2})$. The reciprocal lattice vector $\vec{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2$ with $\mathbf{b}_1 = (1, \frac{\sqrt{3}}{3})$ and $\mathbf{b}_2 = (-1, \frac{\sqrt{3}}{3})$. The model Hamiltonian of the Anderson lattice system we discussed here is defined on this triangular lattice, taking the following form:

$$\begin{aligned}\hat{H} = &-t\sum_{\langle ij\rangle\alpha}(\hat{c}^{\dagger}_{i\alpha}\hat{c}_{j\alpha} + h.c.) + E_d\sum_{i\alpha}\hat{n}_{d,i\alpha} \\ &+ U\sum_i \hat{n}_{d,i\uparrow}\hat{n}_{d,i\downarrow} + \sum_{ij\alpha}(V_{ij}\hat{c}^{\dagger}_{i\alpha}\hat{d}_{j\alpha} + \text{H.c.}) \\ &+ J\sum_{\langle ij\rangle}\hat{\mathbf{S}}_{d,i}\cdot\hat{\mathbf{S}}_{d,j} - \mu\hat{\mathcal{N}}, \end{aligned} \tag{1}$$

where $\hat{c}_{j\alpha}$ and $\hat{d}_{j\alpha}$ are the annihilation operators of the conduction and correlated (or local) electrons [38], respectively, with the subscripts j and α ($=\uparrow, \downarrow$) being the lattice coordinate and the spin index. $\hat{n}_{c,i\alpha}$ and $\hat{n}_{d,i\alpha}$ are the corresponding electron number operators, and $\hat{\mathcal{N}} = \sum_{i\alpha}(\hat{n}_{c,i\alpha} + \hat{n}_{d,i\alpha})$ is the total electron number operator; $\hat{\mathbf{S}}_{d,i} = \frac{1}{2}\sum_{\alpha\alpha'}\hat{d}^{\dagger}_{i\alpha}\vec{\sigma}_{\alpha\alpha'}\hat{d}_{i\alpha'}$ is the spin operator of the local electrons with $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ being the Pauli matrices. The parameter t is the hopping energy of conduction electrons. The parameters E_d, U, and J are for the occupation energy, the Coulomb repulsion, and the spin-spin exchange interaction of local electrons, respectively. In the present study, we assume $t > 0$, $E_d < 0$, $U > 0$, and $J > 0$. Inclusion of finite J in the Hubbard-like model was discussed in the connection with superconductivity [39] and here it ensures the existence of the finite spinon Fermi surface in the absence of Kondo coupling or orbital hybridization as will be illustrated later. Finally, the general orbital hybridization between conduction and local electrons is described by the matrix $\{V_{ij}\}$. It contains both the local (or short-ranged) and nonlocal (or long-ranged) hybridizations. The short-ranged one is denoted by the conventional on-site hybridization parameter $V_{ij} = V$ (when $i = j$), while the long-ranged one is denoted by $V_{ij} = xV$, accounting for the orbital hybridization between the nearest neighboring sites $\langle ij\rangle$. Here, the real parameter x is called the Kondo frustration ratio, measuring the relative strength of the local (short-ranged) and nonlocal (long-ranged) Kondo couplings. The limit of $x \to 0$ recovers the on-site Kondo coupling, and the canonical Anderson lattice model corresponds to the case with $x = 0$ and $J = 0$. We also assume $V_{ij} = 0$ if (i, j) are the further long-ranged conduction-local electron hybridization pairs. As long as $V \neq 0$, the respective numbers of the conduction and local electrons are not individually conserved while their sum remains conserved, so the chemical potential μ is introduced to tune the total electron number.

In the following, we shall solve the Hamiltonian by using the slave rotor technique [40–42]. The slave rotor representation is applied to the local electrons by separating the corresponding charge and spin degrees of freedom such that $\hat{d}_{i\alpha} = \hat{f}_{i\alpha}e^{i\hat{\theta}_i}$, where $\hat{\theta}_i$ ($= \hat{\theta}^{\dagger}_i$) and $\hat{f}_{i\alpha}$ are bosonic and fermionic operators acting on the charge and spin subspaces, respectively. The constraint $\hat{n}_{\theta,i} + \hat{n}_{f,i} = 1$ is enforced to guarantee the equivalence between the local Hilbert spaces spanned by the slave representation and the original one. Here, $\hat{n}_{f,i} = \sum_{\alpha}\hat{f}^{\dagger}_{i\alpha}\hat{f}_{i\alpha}$ is the number operator of the slave fermions (describing the spinons), while $\hat{n}_{\theta,i}$ is the hermitian operator canonically conjugate to the bosonic charge operator $\hat{\theta}_i$, satisfying the relationship $[\hat{\theta}_i, \hat{n}_{\theta,j}] = i\delta_{ij}$.

It is convenient to introduce the Lagrange multiplier λ to implement the constraint by adding the term $\lambda(\hat{n}_{\theta,i} + \hat{n}_{f,i} - 1)$ to the Hamiltonian. Then the model Hamiltonian is rewritten as

$$\begin{aligned}\hat{H} = &\sum_{\vec{k}\alpha}\varepsilon_{c,\vec{k}}\hat{c}^{\dagger}_{\vec{k}\alpha}\hat{c}_{\vec{k}\alpha} + \sum_{ij\alpha}[V_{ij}\hat{c}^{\dagger}_{j\alpha}\hat{f}_{i\alpha}e^{i\hat{\theta}_i} + \text{H.c.}] \\ &+ \left(E_d + \frac{U}{2} - \mu + \lambda\right)\sum_i \hat{n}_{f,i} + J\sum_{\langle ij\rangle}\hat{\mathbf{S}}_{f,i}\cdot\hat{\mathbf{S}}_{f,j} \\ &+ \frac{U}{2}\sum_i \hat{n}^2_{\theta,i} + \lambda\sum_i \hat{n}_{\theta,i}, \end{aligned} \tag{2}$$

where the conduction electron energy is expressed in the momentum space with $\varepsilon_{c,\vec{k}} = -2tX_{\vec{k}} - \mu$ and $X_{\vec{k}} = \cos k_1 + \cos k_2 + \cos(k_1 - k_2)$, keeping track of the symmetry of the triangular lattice. The local electron part is kept in the lattice space and will be treated by the mean field approximation as follows.

III. MEAN-FIELD APPROXIMATION

We expect that Kondo screening develops in the ground state of the Hamiltonian, as in the canonical Anderson lattice system. This is described by the condensation of the hybridization operator $\hat{c}^\dagger_{j\alpha}\hat{f}_{i\alpha}$, represented by the uniform mean field $\chi_{cf} = V^{-1}\sum_{j\alpha} V_{ij}\langle\hat{c}^\dagger_{j\alpha}\hat{f}_{i\alpha}\rangle$ in accordance with the hybridization term in the mode Hamiltonian. Both the local (the on-site $j = i$) and long-ranged (the nearest neighbor sites $\langle ij\rangle$) Kondo hybridizations contribute to the Kondo screening. Notice that χ_{cf} can be chosen as a real order parameter since the phase factor of χ_{cf} can be gauged away by the $U(1)$ transformation. Meanwhile, the charged rotor degrees of freedom participate in the Kondo screening via the operator $e^{i\hat{\theta}_i}$ which appeared in Eq. (2). Such contribution can be described by its condensation on the ground state $\Phi = \langle e^{i\hat{\theta}_i}\rangle$. We treat this parameter as a new mean field which is uniformly valued on the lattice. Then, the hybridization term in Eq. (2) depends on both the mean fields. Assuming that the quantum fluctuations above the mean fields are small, the hybridization term can be decoupled further by using the approximation $\hat{A}\hat{B} \approx \langle\hat{A}\rangle\hat{B} + \hat{A}\langle\hat{B}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle$ for $\hat{A} = \sum_{j\alpha} V_{ij}\hat{c}^\dagger_{j\alpha}\hat{f}_{i\alpha}$ and $\hat{B} = e^{i\hat{\theta}_i}$.

As proposed in theory [29,43,44] and indicated in experiments [45–47], the spin liquid phase driven by the spin exchange interaction is responsible to the spinon Fermi surface state. Such a phase is characterized by the condensation of the spinon bond operator [29], i.e., $\chi_f = \sum_\alpha\langle\hat{f}^\dagger_{i\alpha}\hat{f}_{j\alpha}\rangle$. With this understanding, the spin exchange interaction term can be reexpressed as follows:

$$\sum_{\langle ij\rangle}\hat{\mathbf{S}}_{f,i}\cdot\hat{\mathbf{S}}_{f,j} = -\frac{1}{2}\sum_{\langle ij\rangle}\sum_{\alpha}\hat{f}^\dagger_{i\alpha}\hat{f}_{j\alpha}\sum_{\alpha'}\hat{f}^\dagger_{j\alpha'}\hat{f}_{i\alpha'} - \frac{1}{4}\sum_{\langle ij\rangle}\hat{n}_{f,i}\hat{n}_{f,j} + \frac{Z}{4}\sum_i\hat{n}_{f,i}, \tag{3}$$

where $Z = 6$ is the coordination number of the triangular lattice. After decoupling the rotor and spinon sectors by using the similar approximation, we obtain the following mean-field Hamiltonian:

$$\begin{aligned}\hat{H}_{MF} &= \hat{H}_f + \hat{H}_\theta,\\ \hat{H}_f &= \sum_{\vec{k}\alpha}\begin{pmatrix}\hat{c}^\dagger_{\vec{k}\alpha} & \hat{f}^\dagger_{\vec{k}\alpha}\end{pmatrix}\begin{pmatrix}\varepsilon_{c,\vec{k}} & \Phi V_{\vec{k}}\\ \Phi^* V_{\vec{k}} & \varepsilon_{f,\vec{k}}\end{pmatrix}\begin{pmatrix}\hat{c}_{\vec{k}\alpha}\\ \hat{f}_{\vec{k}\alpha}\end{pmatrix},\\ \hat{H}_\theta &= \sum_i\left(\frac{U}{2}\hat{n}^2_{\theta,i} + \lambda\hat{n}_{\theta,i} + 2V\chi_{cf}\cos\hat{\theta}_i\right).\end{aligned} \tag{4}$$

In the above, $\varepsilon_{f,\vec{k}} = -J\chi_f X_{\vec{k}} + E_d + \frac{1}{2}U + \frac{1}{4}JZ(1-n_f) - \mu + \lambda$ is the dressed spinon energy, $V_{\vec{k}} = V(1 + 2xX_{\vec{k}})$ is the hybridization function in the momentum space, and $n_f = \langle\hat{n}_{f,i}\rangle$ is the average spinon occupation number. Here the $\vec{k}$ dependence of $V_{\vec{k}}$ comes from the coexisting on-site and nearest-neighbor-site hybridizations with x measuring their relative ratio introduced previously. We also assume no spontaneous orbital currents and that the order parameter χ_f is real.

Now, we deal with $\hat{H}_\theta$ using the perturbation theory. Since the rotor sector Hamiltonian is independent of lattice sites, we consider the ith site where the local Hilbert subspace of the rotor sector is spanned by $|m_i\rangle$, the eigenstates of $\hat{n}_{\theta,i}$ with eigenvalues $m_i = 0, \pm1$, satisfying $e^{\pm i\hat{\theta}_i}|m_i\rangle = |m_i \pm 1\rangle$. In the present study, we focus on the boundary of the Kondo phase so that the effective Kondo hybridization $V\chi_{cf}$ is small; the term $2V\chi_{cf}\cos\hat{\theta}_i$ in $\hat{H}_\theta$ is then treated as perturbation. At the zero order, the eigenvalue of the unperturbed part is given by $E(m_i) = (\frac{U}{2}m_i^2 + \lambda m_i)$. We also assume that the Coulomb repulsion is relatively strong so that $U > 2|\lambda|$ is achieved. Hence, the configuration $|m_i = 0\rangle$ is the ground state.

To the first order of $V\chi_{cf}$, the ground state becomes

$$\left|\Psi_0^{(1)}\right\rangle = |0\rangle + \sum_{m_i}\frac{\langle m_i|2V\chi_{cf}\cos\hat{\theta}_i|0\rangle}{E(0) - E(m_i)}|m_i\rangle. \tag{5}$$

Moreover, the expectation values of $e^{i\hat{\theta}_i}$ and $\hat{n}_{\theta,i}$ in this state are respectively given by

$$\Phi = \langle e^{i\hat{\theta}_i}\rangle = -2V\chi_{cf}\left(\frac{1}{U+2\lambda} + \frac{1}{U-2\lambda}\right), \tag{6}$$

$$n_\theta = \langle\hat{n}_{\theta,i}\rangle = (2V\chi_{cf})^2\left[\frac{1}{(U+2\lambda)^2} - \frac{1}{(U-2\lambda)^2}\right]. \tag{7}$$

As expected, Φ is real and $n_f = 1 - n_\theta \neq 1$ if both χ_{cf} and λ are nonvanishing.

Next, we turn to the Hamiltonian $\hat{H}_f$, combining the conduction electrons and the fermionic spinons. This part can be directly solved, resulting in the fermionic quasiparticle dispersions:

$$E^{(\pm)}_{\vec{k}} = \frac{\varepsilon_{c,\vec{k}} + \varepsilon_{f,\vec{k}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{c,\vec{k}} - \varepsilon_{f,\vec{k}}}{2}\right)^2 + (\Phi V_{\vec{k}})^2}. \tag{8}$$

The self-consistent equations for the mean field parameters at zero temperature are given by

$$\chi_{cf} = \frac{1}{2VN}\sum_{\vec{k}\alpha\nu}\nu\Theta\left(-E^{(\nu)}_{\vec{k}}\right)\frac{\Phi V^2_{\vec{k}}}{\sqrt{F(\vec{k})}}, \tag{9}$$

$$\chi_f = \frac{1}{ZN}\sum_{\vec{k}\alpha\nu}\Theta\left(-E^{(\nu)}_{\vec{k}}\right)X_{\vec{k}}\left(1 - \nu\frac{\varepsilon_{c,\vec{k}} - \varepsilon_{f,\vec{k}}}{2\sqrt{F(\vec{k})}}\right), \tag{10}$$

where N is the total number of lattice sites, $E^{(\nu)}_{\vec{k}} = E^{(\pm)}_{\vec{k}}$ for $\nu = \pm1$, respectively, and $F(\vec{k}) = (\frac{\varepsilon_{c,\vec{k}} - \varepsilon_{f,\vec{k}}}{2})^2 + (\Phi V_{\vec{k}})^2$, $\Theta(x)$ is the step function. The occupation constraint is replaced by

$$n_\theta + \frac{1}{2N}\sum_{\vec{k}\alpha\nu}\Theta\left(-E^{(\nu)}_{\vec{k}}\right)\left(1 - \nu\frac{\varepsilon_{c,\vec{k}} - \varepsilon_{f,\vec{k}}}{2\sqrt{F(\vec{k})}}\right) = 1. \tag{11}$$

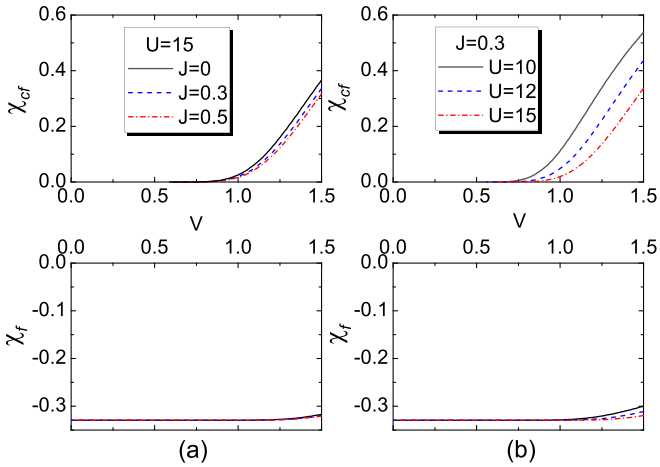

FIG. 2. V dependence of the mean field order parameters with $t = 1$, $E_d = -5$, and $x = 0$ at half filling. (a) for $U = 15$; (b) for $J = 0.3$.

The averaged occupation number of quasiparticles per site, defined by $n = \frac{1}{N}\langle\hat{\mathcal{N}}\rangle$, is given by

$$n = \frac{1}{N}\sum_{\vec{k}\alpha\nu}\Theta\big(-E^{(\nu)}_{\vec{k}}\big). \tag{12}$$

In the following, we shall mainly focus on the case of half-filling, corresponding to $n = 2$. In this case, there is an energy gap, i.e., the Kondo gap, in between $E^{(+)}_{\vec{k}}$ and $E^{(-)}_{\vec{k}}$ when $V\chi_{cf}$ is nonvanishing. We can tune the chemical potential μ such that the Fermi energy is located at the middle of the gap

$$\min E^{(+)}_{\vec{k}} + \max E^{(-)}_{\vec{k}} = 0. \tag{13}$$

With this setting, the mean-field equations, which determine χ_f, χ_{cf}, and λ at zero temperature, become

$$\frac{1}{N}\sum_{\vec{k}}\frac{4\big(\frac{1}{U+2\lambda}+\frac{1}{U-2\lambda}\big)V^2_{\vec{k}}}{\sqrt{(\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}})^2+4(\Phi V_{\vec{k}})^2}} = 1, \tag{14}$$

$$\frac{2}{ZN}\sum_{\vec{k}}\frac{(\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}})X_{\vec{k}}}{\sqrt{(\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}})^2+4(\Phi V_{\vec{k}})^2}} = \chi_f, \tag{15}$$

$$-\frac{1}{N}\sum_{\vec{k}}\frac{\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}}}{\sqrt{(\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}})^2+4(\Phi V_{\vec{k}})^2}} = n_\theta. \tag{16}$$

IV. SOLUTION OF THE SELF-CONSISTENT EQUATIONS

The above set of equations are solved numerically by various choices of the Kondo frustration ratio x while the model parameters $t = 1$ and $E_d = -5$ are fixed. When $x = 0$, the V dependence of the mean field order parameters χ_{cf} and χ_f are shown in Fig. 2. The observations are as follows. First, the spinon hopping order parameter χ_f is negative. Noting that the sign of χ_f cannot be gauged away in the triangular lattice, so in the momentum space the top of the spinon band locates at the bottom of the conduction electron band. Second, χ_f is finite and weakly dependent on V. Third, χ_{cf} as the order parameter for the heavy fermion or Kondo phase is sizably suppressed by U and J. In particular, the competition between the Coulomb interaction and the antiferromagnetic exchange in the formation of the Kondo phase is displayed clearly in the large V regime. Finally, χ_{cf} decreases smoothly to zero with the decrease of V. But the precise location of the critical hybridization V_c where χ_{cf} reaches zero is not sufficiently clear in Fig. 2.

To determine the location of V_c analytically, we let $\chi_{cf} \to 0$ in the mean-field equations. Then Eq. (16) becomes

$$\frac{1}{N}\sum_{\vec{k}}\frac{\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}}}{|\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}}|} = 0. \tag{17}$$

This equation leads to the following condition for the Lagrangian parameter λ:

$$t - \frac{1}{2}J\chi_f = 1.2\left(E_d + \frac{U}{2} + \lambda\right). \tag{18}$$

Meanwhile, χ_f can be solved by Eq. (15) as

$$\chi_f = \frac{2}{NZ}\sum_{\vec{k}}\frac{\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}}}{|\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}}|}X_{\vec{k}} = -0.3294. \tag{19}$$

It is remarkable that this value is independent of any model interaction parameters, reflecting the intrinsic fermionic spinon dispersion on the boundary of the Kondo phase (i.e., $V = V_c$). Meanwhile, according to Eq. (14) we have

$$\frac{1}{N}\sum_{\vec{k}}\frac{4V^2_{\vec{k}}\big(\frac{1}{U+2\lambda}+\frac{1}{U-2\lambda}\big)}{|\varepsilon_{c,\vec{k}}-\varepsilon_{f,\vec{k}}|} = 1. \tag{20}$$

Since the Kondo gap closes on the boundary of the Kondo phase, $\varepsilon_{c,\vec{k}}$ and $\varepsilon_{f,\vec{k}}$ must be degenerate at the Fermi surface when V tends to V_c from the right hand side, i.e., $V \to V_c^+$, the denominator $|\varepsilon_{c,\vec{k}} - \varepsilon_{f,\vec{k}}|$ in the integrand of Eq. (20) has zero points in the $\vec{k}$ space at the continuity limit ($N \to \infty$). In the case of $x = 0$, $V_{\vec{k}}$ is a constant, i.e., $V_{\vec{k}} = V$, the summation over $\vec{k}$ in Eq. (20) diverges unless $V_c = 0$. This result is consistent with the numerical behavior of χ_{cf} plotted in Fig. 2, displaying the exponential suppression behavior of the Kondo effect in the vanishing V limit. So in this case there is no Kondo breakdown transition at finite V.

Now we consider the general situation when the Kondo frustration ratio is finite (nonzero). The hybridization function is then x dependent, $V_{\vec{k}} = V(1 + 2xX_{\vec{k}})$. While the same behaviors of the χ_f and χ_{cf} with increasing U and J are expected for finite x, it is interestingly found that the Kondo phase could break down (i.e., $\chi_{cf} = 0$) at a finite V_c if the Kondo frustration ratio values at a special point, denoted by x_s. Here our observation is that when $x = x_s$, the functions $|\varepsilon_{c,\vec{k}} - \varepsilon_{f,\vec{k}}|$ and $V_{\vec{k}}$ have the same zero points in the $\vec{k}$ space, leading to finite result for the summation in Eq. (20). Specifically, when $\chi_{cf} \to 0$ at the half-filling, $n_f = 1$, we have $|\varepsilon_{c,\vec{k}} - \varepsilon_{f,\vec{k}}| = |(2t - J\chi_f)(1 + 2.4X_{\vec{k}})|$ by using Eq. (18). Hence, a finite V_c exists at $x_s = 1.2$, satisfying

$$\frac{4.8V_c^2\big(\frac{1}{U+2\lambda}+\frac{1}{U-2\lambda}\big)}{t-\frac{1}{2}J\chi_f}\frac{1}{N}\sum_{\vec{k}}|2.4X_{\vec{k}}+1| = 1. \tag{21}$$

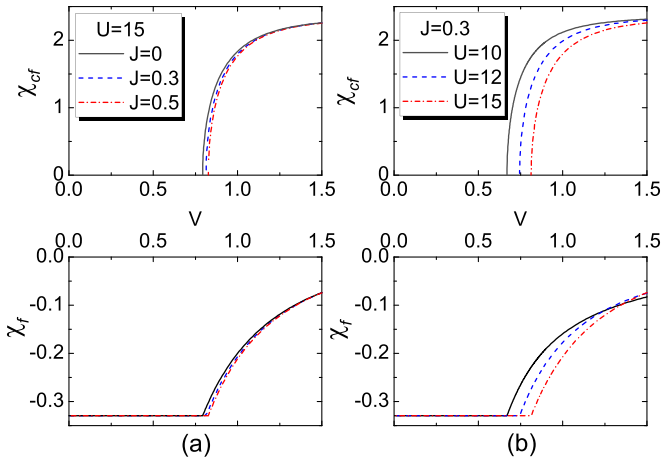

FIG. 3. V dependence of the mean field order parameters with $t = 1$, $E_d = -5$, and $x = 1.2$ at half filling. (a) for $U = 15$; (b) for $J = 0.3$.

Obviously, the summation over $\vec{k}$ is convergent and we can solve the V_c as

$$V_c = 0.35\left[\frac{t'}{U}(t' - 1.2E_d)(1.2U + 1.2E_d - t')\right]^{\frac{1}{2}} \quad (22)$$

with $t' = t + 0.165J$. Using Eq. (18) and the condition $U > 2|\lambda|$, we require $t' < 1.2(U + E_d)$ in order to guarantee a real solution of V_c.

The numerical results for the mean-field order parameters in the case of $x = x_s(= 1.2)$ at half filling are shown in Fig. 3. With the decrease of V, we find that χ_{cf} falls quickly to zero at V_c. For $U = 15$ and $J = 0.5$, $V_c \approx 0.78$, in agreement with the previous analytical estimation. Meanwhile, the magnitude of χ_{cf} becomes larger compared with the case of $x = 0$. This is due to the contribution from the nonlocal Kondo coupling involving six nearest-neighbor hybridizations when $x \neq 0$ (the coordination number $Z = 6$).

Therefore, as long as the Coulomb repulsion (U) of the local electrons is relatively strong, the above analysis indicates the existence of finite χ_{cf} in solving Eq. (14) when $V > V_c$. Otherwise, no real solution for finite χ_{cf} could be found. Hence, V_c is the critical point of the Kondo breakdown quantum phase transition, separating the Kondo insulator phase and the local moment spin liquid phase, the latter being dynamically (or effectively) decoupled from the conduction electrons. On the other hand, when U is relatively small, such that $U < U_0$ with $U_0 \equiv 2\lambda(= 0.835t' - E_d)$, the ground state configuration of the rotor sector is $|m_i = -1\rangle$. In this case, the occupation number per site of the correlated electrons approaches two, the Kondo screening does not take place, and the system is in the conventional Fermi liquid phase.

The quantum phase diagram at half filling with $x = x_s(= 1.2)$ is illustrated in Fig. 4. There are three regions: (i) when $U < U_0(\equiv 0.835t' - E_d)$, the system is in the conventional Fermi liquid phase (FL); (ii) when $U > U_0$ and $V < V_c$ (V_c is denoted by the curve in Fig. 4), $\chi_{cf} = 0$ and $\chi_f \neq 0$, the system is in the decoupled local moment spin liquid phase (SL); (iii) in the remaining region of the phase diagram, $\chi_{cf} \neq 0$, the system is in the Kondo insulator phase (KI).

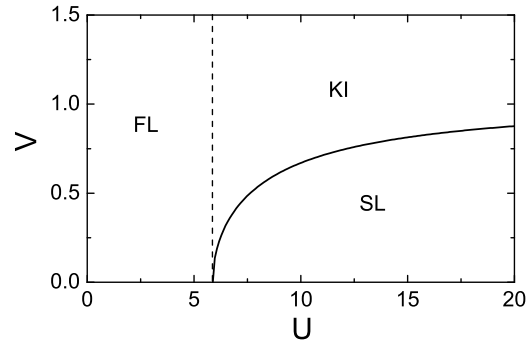

FIG. 4. The quantum phase diagram at half filling. The model parameters are chosen as $t = 1$, $E_d = -5$, $J = 0.3$, and $x = 1.2$.

Finally, it is interesting to notice, as we have already observed above, that the existence of a finite V_c depends not only on the Kondo frustration ratio x, but also on the filling factor of conduction electrons, i.e., $n_c = \langle\sum_\alpha \hat{n}_{c,i\alpha}\rangle$, which is tunable by the chemical potential μ. Previous analysis shows that at $n_c = 1$ the corresponding x_s is 1.2, meaning that as long as x is away from x_s, there is no nonzero V_c and the Kondo screening effect is robust. It is in this sense that the spin liquid phase is also critical in the parameter space of x. To seek for the explicit dependence of x_s on the electron filling, we set $\chi_{cf} = 0$ and solve the equations (9)–(11) again, obtaining the filling dependence of the x_s as shown in Fig. 5 where the horizontal axis represents n_c. We find that x_s is always nonzero for any $0 < n_c < 2$ as previously expected. Moreover, x_s is negative or positive when $n_c < 0.81$ or $n_c > 0.81$, respectively, while it is divergent at $n_c = 0.81$. The divergent x_s corresponds to the limit of the strong frustration where the on-site hybridization strength is vanishingly small. In the relevant bulk or layered materials it is reasonable to expect $|x| < 1$, so the corresponding x_s may be realized at the low or high electron filling regimes.

For instance, when $n_c = 0.5$ (or $n_c = 1.3$), the corresponding special point is given by $x_s = -0.64$ (or $x_s = 0.57$), the absolute magnitude $|x_s|$ is significantly smaller than one. This Kondo frustration ratio seems accessible in the relevant materials. By extending the previous calculations as plotted in Fig. 4, we can obtain the corresponding results for the U-dependent critical hybridization, $V_c(U)$, for other band fillings. In Fig. 6, the curves $V_c(U)$ for several typical values of electron filling ($n_c = 0.5$ and $n_c = 1.3$ with the corresponding

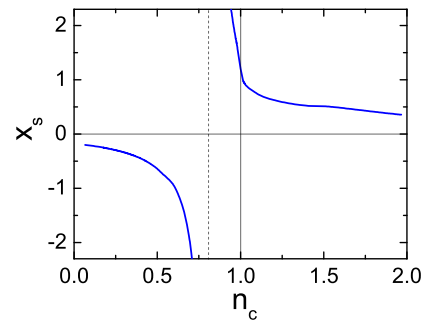

FIG. 5. The conduction electron filling dependence of the Kondo frustration ratio x_s for the existence of finite V_c.

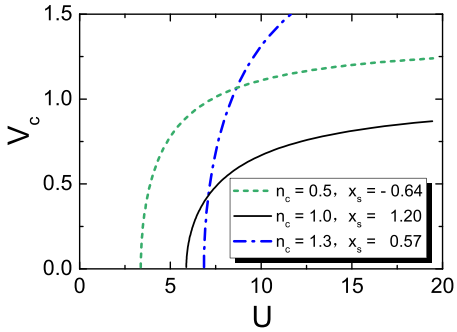

FIG. 6. The critical lines for the three representative band fillings with the corresponding x_s.

x_s mentioned above) are plotted together with the previous result of $n_c = 1$. It is found that the threshold value U_0 where $V_c(U_0) = 0$ increases with the band filling. It should be also noticed that for the band filling $n_c \neq 1$, while the Fermi liquid ($U < U_0$, $V_c = 0$) and the local moment spin liquid ($U > U_0$ and $V < V_c$) phases persist, the region enclosed by $U > U_0$ and $V > V_c$ is the heavy fermion phase with a large Fermi surface.

V. CONCLUSION AND DISCUSSION

Summarizing, we have investigated a periodic Anderson-Heisenberg triangular lattice model system with both geometric and Kondo frustrations. In addition to the conventional Fermi liquid phase and the Kondo (or heavy fermion) phase, a dynamically decoupled local moment spin liquid phase is found in the quantum phase diagram in terms of the Coulomb repulsion U and the Kondo hybridization V. Such a phase depends critically on the Kondo frustration ratio x, thus termed as the critical spin liquid phase which is absent in the canonical Anderson triangular lattice without the Kondo frustration ($x = 0$). For a given system with the fixed Kondo frustration, tuning the electron filling can shift the nodal points of the hybridization function $V_{\vec{k}}$ to the Fermi level, leading to the transformation of Fermi surfaces in the spin liquid phase at a finite V_c below which the Kondo screening effect breaks down.

The physical implication of the $\vec{k}$-dependent hybridization function was previously discussed in connection with the momentum-dependent Fermi surface reconstruction and anisotropic Kondo gap observed in some relevant heavy fermion compounds [48–51], while the appearance of nodes in $V_{\vec{k}}$ has not been adequately explored except for a few cases in connection with the unconventional Fermi liquid [52] and topological Kondo insulator [53]. The present study reveals a new physical consequence of the hybridization nodes, namely the possible critical spin liquid phase in the layered Kondo triangular lattice systems. Here the spin liquid feature is characterized by the nonvanishing condensation parameter χ_f based on the slave-rotor decoupling approach. We notice that the mean-field method may overestimate the condensation tendency, the influence of quantum fluctuations above the mean-field level on this phase remains open and deserves further investigations. Nevertheless, the geometric frustration due to the triangular lattice symmetry and the Kondo frustration in the discussed model system could further enhance the stability of the spin liquid phase.

Associated with this phase is the formation of the spinon Fermi sea formed by the fermionic quasiparticles [35–37] with the hopping amplitude $\frac{1}{2}J\chi_f$. While in the heavy fermion phase, the corresponding Fermi surface should be larger due to the contributions from both conduction electrons and fermionic spinons. This allows us to predict the transition from the critical spin liquid phase to the heavy fermion phase in experiments by tuning some physical parameters, including the electron filling factor (or carrier density) as well as the Kondo coupling (or hybridization strength). Of course, the tunability of the electron density and Kondo coupling in the bulk f electron materials, which is usually realized by physical pressure and chemical substitution, remains an experimental challenge.

Remarkably, such tunability can be realized by tuning the electric field and gate voltages in the synthetic Anderson (or Kondo) lattices such as the transition metal-dichalcogenide bilayer heterostructures 1T-$TaSe_2$/1H-$TaSe_2$ [21] and $MoTe_2$/WSe_2 [54]. In particular, the Kondo frustration ratio at which the finite V_c exists can be reached in a wide region of the electron doping n_c as shown in Fig. 5. Therefore, we expect that tuning the electric field and gate voltages in the bilayer heterostructures could tune the hybridization magnitude across the critical point, resulting in the changes in Fermi surfaces and heavy fermion behavior. These features can be probed in various transports, quantum oscillations, as well as specific heat measurements. Another class of the material's candidate to observe the variable hybridization and spin liquid feature is the rare earth intercalated bilayer graphene where the density of f electrons can be tuned by the rare earth doping [55,56].

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