I. INTRODUCTION

Since the pioneering proposal by Anderson [1], there has been an extensive quest to find quantum spin liquids (QSL) in materials [2–4]. Recently, it has been suggested that certain layered transition metal dichalcogenide compounds might harbour a QSL state [5, 6]. In particular, 1T-TaS$_2$, a material that undergoes a commensurate charge density wave transition around 200K into a $\sqrt{13} \times \sqrt{13}$ star of David structure [7, 8], remains insulating to the lowest temperatures in spite of having an odd number of electrons per star of David supercell, and yet shows no sign of any further conventional ordering phase transition such as antiferromagnetism that would double the unit cell, to the lowest measurable temperatures [9]. The magnetic susceptibility of this compound remains nearly constant at low temperatures [10] and the material displays a finite linear in temperature specific heat coefficient [11] indicative of a finite density of states at low energies. Earlier experiments found no linear in temperature heat conductivity [12], which was taken as evidence against itinerant carriers, but more recent experiments have shown a delicate sensitivity of heat transport to impurities [13], finding a finite linear in temperature heat conductivity in the cleanest samples indicative of the presence of a finite density of states of itinerant carriers, as expected for the spinon fermi surface state. Moreover, band structure analysis [14] showed that a single narrow band crosses the Fermi energy and is separated from other bands, making it very likely that the low energy electronic behaviour can be described by a single band Hubbard model.

A closely related compound, 1T-TaSe$_2$ which also undergoes a commensurate charge density wave transition into the star of David structure is expected to display similar phenomenology. While bulk 1T-TaSe$_2$ is metallic [15], monolayer 1T-TaSe$_2$ was studied by STM and found to be a Mott insulator [16]. Recently Crommie and coworkers [17] extended their study by placing a monolayer of 1T-TaSe$_2$ on top of a 1H-TaSe$_2$ monolayer which is metallic. Surprisingly their experiment has found that a Kondo-like resonance peak near the Fermi energy develops in the tunnelling density of states. It is important to emphasize that in these experiments the tunnelling tip is coupled primarily to the originally insulating top layer of 1T-TaSe$_2$, and therefore, taken at face value, the appearance of a tunnelling density of states peak near zero bias may imply the destruction of the presumed spin liquid that would exist for 1T-TaSe$_2$ in isolation and the formation of a coherent metallic state by the coupling with the substrate metallic 1H-TaSe$_2$, as it would be expected the classic problem of Kondo heavy metal formation.

These experimental findings motivate us to consider a model consisting of a layer of correlated electrons coupled to a layer of non-interacting itinerant electrons via tunnelling to study the competition of spinon fermi surface states and the heavy Kondo metals. There are two questions that we would like to address. First, the experimentalists found an excellent fit of the lineshape and its temperature dependence with that expected for the Kondo resonance of a single impurity Kondo problem [17]. On the other hand, the actual system consists of a periodic array of local moments. Even if we are in the Kondo limit, the low temperature state is expected to be a heavy Fermion metal. Would the formation of a narrow coherent band lead to observable changes in the local density of states? Second, how does the Heisenberg exchange coupling $J_H$ between the local moments compete with the Kondo coupling $J_K$ that operates between the local moments and the conducting substrate?
This problem was considered by Doniach [18] for the case when the Heisenberg coupling leads to an antiferromagnetic state. His conclusion is that two relevant competing energy scales are the Kondo temperature $T_K$ and the Heisenberg exchange scale $J_H$. Note that at weak coupling $T_K$ is exponential small in terms of the Kondo coupling $J_K$. This would suggest that a very weak $J_H$ is sufficient to destroy the Kondo effect. If the experiment were interpreted as being in the Kondo limit, this places a rather small upper bound on $J_H$ of about 50K, since the scale $T_K$ is estimated to be about 50K from the experimental fit [17]. With such a small Heisenberg coupling, the interpretation of the monolayer 1T-TaSe$_2$ as a spin liquid is brought into question. We note that the situation may change when the coupling becomes strong, and it may also change in frustrated spin models where the spin liquid state may be favored over the anti-ferromagnet. Recall that in the resonating valence bond (RVB) picture, the quantum spin liquid is viewed as the superposition of singlet formed between local moment pairs, while the Kondo phenomenon arises from the singlet formation between the local moment and the conduction electron spin. The competition between different ways of forming singlets may well be different from the competitive spin liquid layer, which hop with an amplitude ($V$) for the correlated electrons that reside in the putative metallic layer, while the correlated electrons are viewed as the “itinerant”, and those created by $d^i$ are represented by a bosonic rotor, $\theta_i$, and a fermionic spinon $f_{i,\sigma}$ degrees of freedom: $d_{i,\sigma} \equiv e^{i\theta_i} f_{i,\sigma}$, with the constrain $n_{\theta,i} + n_{f,i} = 1$. The Hamiltonian can be written as:

$$H = - t_d \sum_{\langle i,j \rangle, \sigma} d_{i,\sigma}^\dagger d_{j,\sigma} + \sum_i n_{d,i} (\epsilon_d^{(0)} - \mu_F)$$

$$- t_c \sum_{\langle i,j \rangle} c_{i,\sigma}^\dagger c_{j,\sigma} + \sum_i n_{c,i} (\epsilon_c^{(0)} - \mu_F)$$

$$+ \frac{U}{2} \sum_i (n_{d,i} - 1)^2 - V \sum_{i,\sigma} (c_{i,\sigma}^\dagger d_{i,\sigma} + h.c.).$$

(1)

Our paper is organized as follows: Section II sets up the model and describes the mean-field slave rotor approach that we employ to tackle it. Section III presents the solution of this mean field under a wide range of parameters, including not only the interplay between spinon fermi surface and heavy metal but also the possibility of competing with Kondo insulating states. Section IV is devoted to a detailed analysis of the LDOS spectra and temperature dependence of the LDOS width and the comparison with STM experiments. Section V summarizes and further discusses our main findings. We have relegated some of the technical details of the mean field treatment to Appendix A. Appendix B reviews the classic result of the temperature dependence of the single impurity Anderson model and points out a correction to the width of the Kondo resonance that has been missed in previous interpretations of experiments (compare Eq. (B5) and Eq. (B7)).

II. MODEL AND SLAVE ROTOR APPROACH

We consider a model of two-species of fermions residing in a triangular lattice that interpolates naturally between the Hubbard model and the periodic Anderson model, the microscopic Hamiltonian of the system has the form:

Here the electrons created by $c^\dagger$ are viewed as the “itinerant”, and those created by $d^\dagger$ as the correlated ones. In the limit in which the correlated electrons are localized, $t_d = 0$, this model reduces to the periodic Anderson model and in the limit in which the two species are decoupled, $V = 0$, the Hamiltonian for the correlated electrons reduces to the Hubbard model. We would like to employ a formalism capable of handling the various regimes of this model, and in particular the single occupancy constraints that appear in the large $U$ limit. For this purpose we resort to the slave rotor mean-field approach. According to the slave rotor method [21, 24], the $d$-electron can be represented by a bosonic rotor, $\theta_i$, and a fermionic spinon $f_{i,\sigma}$ degrees of freedom: $d_{i,\sigma} \equiv e^{i\theta_i} f_{i,\sigma}$, with the constrain $n_{\theta,i} + n_{f,i} = 1$. The Hamiltonian can
be then written in terms of these partons as follows:

\[
H = -td e^{-i\theta_i} e^{i\theta_j} \sum_{(i,j),\sigma} f_{i,\sigma}^\dagger f_{j,\sigma} + \sum_i n_{f,i} (\epsilon_{d}^{(0)} - \mu_F)
- t_c \sum_{(i,j),\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + \sum_i n_{c,i} (\epsilon_{c}^{(0)} - \mu_F)
+ \frac{U}{2} \sum_i n_{\theta,i}^2 - V \sum_{i,\sigma} (e^{i\theta_i} c_{i,\sigma}^\dagger f_{i,\sigma} + h.c.).
\] (2)

A. Mean-field theory

In the spirit of a mean-field theory we approximate the ground state of Eq. (2) by a direct product of a rotor state and a spinon state. The constrain on the rotor and spinon occupation is satisfied on average:

\[
\langle n_{\theta,i} \rangle + \langle n_{f,i} \rangle = 1,
\] (3)

since the rotor and spinon degrees of freedom are assumed to be disentangled, we write down the mean-field Hamiltonian as the sum of a rotor part and a purely fermionic part, i.e., \( H_{\text{mfl}} = H_f + H_\theta \), with

\[
H_f = -T_f \sum_{(i,j),\sigma} f_{i,\sigma}^\dagger f_{j,\sigma} + \sum_i n_{f,i} (\epsilon_{d}^{(0)} + \lambda - \mu_F)
- t_c \sum_{(i,j),\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + \sum_i n_{c,i} (\epsilon_{c}^{(0)} - \mu_F)
- V_f \sum_i c_{i,\sigma}^\dagger f_{i,\sigma} + h.c.,
\] (4a)

\[
H_\theta = -2T_\theta e^{-i\theta_i} e^{i\theta_j} + \sum_i \frac{U}{2} n_{\theta,i}^2 + \lambda n_{\theta,i} - 4V_\theta \cos(\theta_i),
\] (4b)

\[
T_f = t_d (e^{-i\theta_i} e^{i\theta_j})_\theta,
\] (4c)

\[
V_f = V (e^{i\theta_i})_\theta,
\] (4d)

\[
T_\theta = t_d (f_{i,\sigma}^\dagger f_{j,\sigma})_f,
\] (4e)

\[
V_\theta = V (c_{i,\sigma}^\dagger f_{i,\sigma})_f,
\] (4f)

here a Lagrange multiplier \( \lambda \) is introduced to maintain the constrain Eq. (3). The quasiparticle residue of correlated \( d \) electron is \( \langle e^{i\theta_i} \rangle \neq 0 \) and can be regarded as the order parameter for the metallic phase, when its value is finite, there will be a coupling between the spinon and itinerant electrons. In this work, we will concentrate on the competition of this correlated metallic state and a more exotic state, known as the spinon fermi surface state, that arises when \( \Phi = 0 \) and the spinon, \( f \), has a fermi surface.

We simplify the electronic part and approximate the band structure for spinons (\( f \)) and itinerant electrons (\( c \)) by simple parabolic bands:

\[
H_f = \sum_{k,\sigma} f_{k,\sigma}^\dagger f_{k,\sigma} + c_{k,\sigma}^\dagger c_{k,\sigma} - V_f \left(\epsilon_{c,\sigma}^\dagger f_{k,\sigma} + h.c.\right),
\] (5a)

\[
\epsilon_{f,k} = \frac{3}{2} T_f \left( k^2 - \frac{\Lambda^2}{2} \right) + \lambda - \mu_F,
\] (5b)

\[
\epsilon_{c,k} = \frac{3}{2} t_c \left( k^2 - \xi \Lambda^2 \right) - \mu_F,
\] (5c)

here the \( \Lambda \) is a cut-off of the \( k \)-space intended to mimic the finite size of the Brillouin zone which can be determined by equalling \( \pi \Lambda^2 \) to the area of triangular lattice’s Brillouin zone. The parameter \( \xi \) in \( \epsilon_{c,k} \) reflects the occupancy of \( c \) electrons when \( c \) and \( f \) fermions are decoupled (since in such case \( \lambda = 0 \) and \( \mu_F = 0 \), see discussion in the following section): the number of \( c \) electron per site is \( \xi \) when the dispersion \( \epsilon_{c,k} \) is particle like with \( t_c \) being positive, and \( 2 - \xi \) with hole like dispersion (negative \( t_c \)).

The reason for this simplification is that we expect that the essential aspects of the physics are not sensitive to the detailed form of the band dispersion, thus in this study we simply take the bands as in Eq. (5b), which greatly simplifies the analytic treatment.

B. Expectation values of the rotor operators

Notice that even after the mean field decoupling, the rotor Hamiltonian \( H_\theta \) is still essentially a 2D quantum XY model with a transverse field which is not amenable to analytic treatment. Therefore, one has to make further approximations.

We are interested in solutions that respect time-reversal and translational symmetry and that have no flux per unit cell. Therefore we seek for self-consistent solutions where \( \Phi \) is uniform and real. To do so, we perform an additional self-consistent mean-field treatment of \( H_\theta \) by introducing an effective single-site rotor Hamiltonian:

\[
H_\theta^{(1)} = -K_\theta (e^{i\theta} + e^{-i\theta}) + U \frac{n_{\theta}^2}{2} + \lambda n_{\theta},
\] (6a)

\[
K_\theta = 2zT_\theta \Phi + 2V_\theta,
\] (6b)

with \( z \) being the lattice coordination (\( z = 6 \) for triangular lattice). To lowest order in perturbation theory in \( K_\theta/U \) (\( \lambda = 0 \) since we are interested in half-filled spinon and the constrain Eq. (3) leads to \( \langle n_{\theta,i} \rangle = 0 \) we have \( \Phi = 4K_\theta/U \). On the other hand, in the opposite limit in which \( K_\theta/U \gg 1 \), we have \( \theta \approx 0 \) and thus \( \Phi = \langle e^{i\theta} \rangle = 1 \). Moreover, since \( \Phi = \langle e^{i\theta} \rangle \) is never greater than one, we introduce the following natural interpolation between these limits:

\[
\Phi = \frac{K_\theta}{\sqrt{(U/4)^2 + K_\theta^2}},
\] (7)
or equivalently,
\[ K_{\theta} = \frac{U}{4} \frac{\langle e^{i\theta} \rangle}{\sqrt{1 - \langle e^{i\theta} \rangle^2}}, \]  
(8)

Although the above mean field treatment captures well the behavior of the residue \( \Phi \), it ignores completely the nearest neighbour rotor correlations, which are essential in order to obtain a dispersion for the spinon. To capture these, and since \( V_{\theta} \) is small near the metal to insulator phase transition, we will approximate their value by performing a perturbative calculation directly with the more complete rotor Hamiltonian \( H_{\theta} \) from Eq. (4b), which contains the \( U \) and \( T_{\theta} \) terms only,
\[ \tilde{H}_{\theta} = \frac{U}{2} \sum_i n_{\theta,i}^2 - 2T_{\theta} \sum_{(i,j)} e^{-i\theta_i} e^{i\theta_j}, \]
(9)
which leads to the following nearest neighbor rotor correlations:
\[ \langle e^{-i\theta_i} e^{i\theta_j} \rangle \approx \frac{4T_{\theta}}{U}, \]
(10)
it should be noted that these nearest-neighbor rotor correlations from Eq. (10) are needed to reproduce the spinon bandwidth which is expected to be given by the Heisenberg exchange coupling scale \( J_H = 4t_d^2/U \). The expressions above are all zero temperature results. The finite temperature version of these formulae are discussed in Appendix A.

C. Expectation values of the fermion operators

The fermionic mean-field Hamiltonian is free from interactions and can be diagonalized exactly. Because we are already accounting for spinon hopping in the spin liquid phase at \( V = 0 \), the correlator \( \langle f_{i,\sigma}^\dagger f_{j,\sigma} \rangle \) is not expected to change much during the spin-liquid to heavy-metal phase transition, so we will simply approximate its value when \( c \) and \( f \) fermions are decoupled from each other (\( V_f = 0 \) in the insulating phase):
\[ \langle f_{i,\sigma}^\dagger f_{j,\sigma} \rangle = \frac{1}{N} \sum_k \delta_{k,i,j} n_F(\epsilon_f,k) \equiv \chi_0, \]
(11)
with \( n_F \) being the Fermi-Dirac distribution function:
\[ n_F(x) = \frac{1}{e^{\beta x} + 1}, \]
thus \( T_{\theta} = t_d \chi_0 \). As for the hybridization between the itinerant electrons and spinons, one obtains:
\[ \langle c_{i,\sigma}^\dagger f_{i,\sigma} \rangle = V_f \chi_{cf}, \]
(12a)
\[ \chi_{cf} = -\frac{1}{2N} \sum_k \frac{n_F(E_{1,k}) - n_F(E_{2,k})}{\sqrt{\left(\frac{\epsilon_f,k - \epsilon_{c,k}}{2}\right)^2 + V_f^2}}, \]
(12b)
with quasi-particle energy dispersions:
\[ E_{1/2,k} = \frac{\epsilon_f,k + \epsilon_{c,k}}{2} \pm \sqrt{\left(\frac{\epsilon_f,k - \epsilon_{c,k}}{2}\right)^2 + V_f^2}, \]
(13)
and the occupancy of spinon reads:
\[ \langle f_{i,\sigma}^\dagger f_{i,\sigma} \rangle = \frac{1}{N} \sum_k \cos^2(\alpha_k) n_F(E_{1,k}) + \sin^2(\alpha_k) n_F(E_{2,k}), \]
(14a)
\[ \cos(2\alpha_k) = \frac{\epsilon_f,k - \epsilon_{c,k}}{2} \sqrt{\left(\frac{\epsilon_f,k - \epsilon_{c,k}}{2}\right)^2 + V_f^2}, \]
(14b)

D. Self-consistent equations

Once the expressions for the expectation values of the rotor and fermions are obtained, the self-consistent equations for the order parameter \( \Phi \) can be derived, from Eqs. (6b), (8) and (12a), one can easily show that:
\[ \frac{\Phi}{8} \left( \frac{1}{\sqrt{1 - \Phi^2}} - 8z t_d U \chi_0 \right) = \frac{V^2}{U} \chi_{cf}, \]
(15)
so one needs to solve Eq. (15) along with the constrain Eq. (3) and \( \langle n_{f,i} \rangle = 1 \). It is obvious that Eq. (15) always has a trivial solution \( \langle e^{i\theta} \rangle = 0 \), and the non-trivial solution of \( \langle e^{i\theta} \rangle \) satisfies:
\[ \frac{1}{8} \left( \frac{1}{\sqrt{1 - \Phi^2}} - 8z t_d U \chi_0 \right) = \frac{V^2}{U} \chi_{cf}. \]
(16)
It should be noted that the “susceptibility” \( \chi_{cf} \) also depends on \( \Phi \) in general.

III. MEAN-FIELD PHASE DIAGRAM AND MEAN-FIELD PROPERTIES.

To explore the phase transition between the spin liquid and heavy metal phases, it is important to distinguish the cases with the band dispersions of the \( d \)-electron and itinerant electrons being particle-particle like (\( t_d > 0 \) and \( t_c > 0 \)) and particle-hole like (\( t_d < 0 \) and \( t_c < 0 \)). Here we discuss in detail the behavior when the itinerant fermion has higher density (larger fermi surface area) than the spinon, which is most relevant to the recent experiments 1T-TaS\(_2\) and 1T-TaSe\(_2\), and for \( 1 \leq \xi < 2 \) for the particle-particle case and \( 0 \leq \xi < 1 \) for the particle-hole case (one will see that this leads to \( n_c \geq n_f \) in the insulating phase), the results for the complementary regime will be qualitatively the same.

A. Particle-particle dispersion

In this section, we discuss the situation for particle-particle like dispersions. As mentioned before, two competing phases in our phase diagram: the spin liquid phase and the heavy metal phase (see Fig. 4 for an example of the phase diagram). The phases are determined by whether order parameter \( \Phi \) is finite (heavy metal) or not.
(spin liquid). When $t_d \sim 0$, the model reduces to a periodic Anderson model and the transition from spin liquid to heavy metal is of the form of a weak coupling instability. On the other hand, for larger $t_d/U \sim 1/8$ and $V = 0$, the system exhibits a metal-insulator (Mott) transition, as one naturally expects from a Hubbard model.

The goal of next section is to see how the phase boundary evolves between these two regimes.

1. Phase boundary

As mentioned above, the phase boundary is obtained when $\Phi = 0$ is a solution of Eq. (16). According to the constrain from Eq. (3) and $(n_{f,i}) = 1$, we have that $(n_{g,i}) = 0$. This leads to a value $\lambda = 0$ for the Lagrange multiplier in Eq. (4b). Thus one just need to self-consistently adjust the chemical potential $\mu_F$ such that the spinon is half-filled. Along the phase boundary, since $c$ and $f$ fermions are decoupled, this can be satisfied by setting $\mu_F = 0$, which leads to $n_{f,i} = 1$ and $n_{c,i} = \xi$, which corresponds to two Fermi surfaces from the two bands with Fermi momentum $k_{F,f} = \Lambda/\sqrt{2}$ and $k_{F,c} = \Lambda\sqrt{2}/2$. In this case the susceptibility of $c$-$f$ coupling reads as:

$$\chi_{cf}^{(0)} = -\frac{1}{N} \sum_k n_F(\epsilon_{f,k}) - n_F(\epsilon_{c,k})$$

$$= \frac{1}{2} \frac{2}{}\Lambda^2 \frac{1}{3} \ln \left( \frac{T_f}{T_c} \right).$$

(17)

It is interesting to notice that the $\chi_{cf}^{(0)}$ is independent of $\xi$ or, in other words, the density of itinerant electrons in this case. This implies that the phase boundary is insensitive to the $c$ electron’s density within the parabolic band approximation. The critical value at which the residue $\Phi$ and the hybridization between the itinerant and correlated electron, $V_f$, become simultaneously non-zero is given by:

$$\frac{V^2}{U} = \frac{1}{8} \left( 1 - 8z \tau \frac{t_d}{t} \right)^2 F^{2} \ln \left( \frac{4 \sqrt{2} T_c}{t_d} \right).$$

(18)

A plot of the phase boundary in this case can be found in Fig. 2(a). As it approaches the Anderson ($t_d \sim 0$) limit, the critical $V^2/U$ has a logarithmic dependence on $t_d/U$. This means that in the local moment limit, the heavy fermion liquid phase is destabilized by a weak Heisenberg coupling, $J_H \sim t_d/U$, comparable to the Kondo scale, $T_K \sim e^{-1/J_K}$ (with $J_K \sim V^2/U$). This is responsible for the sharp narrowing of the region of the Heavy fermi liquid phase in the local moment limit $V^2 \ll t_d/U$, and $t_d \ll U$, as shown in Fig. 2(a). Around the axis $V = 0$ we recover the physics of the spin-liquid to metal (Mott transition) in the conventional Hubbard model on a triangular lattice and the transition occurs at $t_d/U \sim 1/8$, which is in line with previous cluster mean-field calculation [24].

2. Turning on of the heavy fermion phase

As one enters the heavy fermion metallic phase ($\Phi$ becomes finite), both the $E_{1,k}$ and $E_{2,k}$ bands cross the Fermi level (as indicated by the green dashed lines in Fig. 1(a)). According to Eq. (14a), the spinon density in this case is:

$$\langle f_{i,\sigma}^\dagger f_{i,\sigma} \rangle = \frac{k_{F1}^2 + k_{F2}^2}{2A^2} + \frac{\sum_{\alpha=c,f} \epsilon_{\alpha,k_1} + \epsilon_{\alpha,k_2}}{3A^2(T_c - T_f)},$$

by requiring this to be $1/2$, one can obtain $\mu_F = 0$ (with $\lambda = 0$). It can be shown that in this case, the susceptibility...
is simply a constant:

$$\chi_{cf} = \frac{2}{3} \frac{1}{\Lambda^2} \ln(\frac{4t_d^2\chi_0}{Ut_c}) \tag{20}$$

Notice that $\chi_{cf}$ is independent of $V_f$ (or $\Phi$), which is a consequence of the parabolic model. Physically $\chi_{cf}$ should be a monotonic decreasing function of $V_f$ for a general band dispersion, but we conclude from the above that it is weakly dependent on these parameters whenever the bands can be approximated by parabolas. Nevertheless, Eq. (20) still unveils an important effect of the correlated fermion hopping $t_d$, which is to set a “cut-off” to the $\chi_{cf}$ which is otherwise absent in the pure periodic Anderson model and leads to the well-known divergence of this. In the Anderson/atomic limit ($t_d \to 0$), we would have that $\chi_{cf} \to \infty$ as $V_f \to 0$, which is associated with a weak-coupling (Kondo) instability leading to the formation of the heavy fermi liquid state.

On the other hand, there is a further phase transition that appears within the heavy fermi liquid state, associated with the disappearance of one of the fermi surfaces while preserving the net Luttinger volume, at large $V_f$. This occurs when $V_f$ is larger than some critical value $V_f^* = \frac{\Lambda^2}{6} \sqrt{T_f} \frac{t_c}{2} - 2^2$, for which we have that $E_{2,\Lambda} < 0$, so the $E_{1,k}$ band is fully occupied and there is only one Fermi surface associated with the band $E_{1,k}$ (see yellow dashed lines in Fig. 1(a)). In this case, the density of spinon reads:

$$\langle f_i^{\dagger} f_i \rangle = \frac{k_F^2 + \Lambda^2}{2\Lambda^2} + \frac{\epsilon_{f,k_F} + \epsilon_{c,k_F} + \sqrt{(\epsilon_{f,\Lambda} - \epsilon_{c,\Lambda})^2 + 4V_f^2}}{3\Lambda^2(t_c - T_f)} \tag{21}$$

and the $\mu_F$ can be determined by requiring $\langle f_i^{\dagger} f_i \rangle = 1/2$. In this case the susceptibility $\chi_{cf}$ is no longer independent of $V_f$ (we do not show the explicit expression here since it is too lengthy). Fig. 2(b) shows a plot the $\chi_{cf}$ as a function of $V_f$ for a specific parameterization. As mentioned before, a finite $t_d$ sets a “cut-off” to the $\chi_{cf}$, moreover, the critical $V_f^*$ will also decrease as $t_d$ decreases. So in the Anderson/atomic limit where $t_d = 0$, the plateau region of $\chi_{cf}$ will disappear and it diverges as $V_f \to 0$, which will result in a weak-coupling instability to a heavy metal (or the so-called heavy fermion) phase. This role of $t_d$ as a cutoff of the susceptibility for hibridization of correlated and itinerant electrons is what leads to an increasing value of the critical $V_f$ to transition into the heavy fermion liquid state as $t_d$ increases, as shown in Fig. 2(a) at extremely small values of $t_d$. In other words, the larger the value of $t_d$ the smaller the susceptibility to induce the mixing between the itinerant and correlated fermions.

However, the physical role of $t_d$ is not exclusively to cutoff $\chi_{cf}$, as it is clear from the Fig. 2(a) that eventually at sufficiently large $t_d$ the critical $V_f$ starts to decrease as $t_d$ increases. The other physical role of $t_d$ can be understood from the self-consistent equation for the residue $\Phi$, Eq. (16), where we see that the hopping of correlated electrons $t_d$ appears not only inside $\chi_{cf}$, but also on the left hand side of the equation, arising from the coupling between nearest neighbour rotors in $H_0 (t_d e^{-i\theta} e^{i\theta})$. This term competes with the interaction part ($\sim U n_{f}^{2}$) and tends to “lock” the angles of nearby rotors, therefore, in this second role, $t_d$ tends to enhance the appearance of a residue and therefore favors the destruction of the spin liquid in favor of the appearance of the finite $\Phi$.

To illustrate more concretely these contrasting roles of $t_d$ we compare the solution of $\Phi$ as a function of $V_f^2/U$ for different types of modified self-consistent equations. As shown by the dashed curves in Fig. 3, when the susceptibility $\chi_{cf}$ is replaced by one which diverges logarithmically at small $V_f$ (dashed lines), there is always a weak-coupling instability to the heavy fermion phase, while for the exact $\chi_{cf}$ (solid lines), one has to reach a finite critical value of $V_f$ for the occurrence of the heavy metal phase. Moreover, when the linear $t_d$ terms from the left hand side of Eq. (16) is removed (blue lines), the heavy metal phase is also suppressed and one needs a larger $V_f$ to get a non-zero $\Phi$.

From the analysis above, one can see that either a very large $t_d$ (nearby rotors lock strongly) or a very small $t_d$ (susceptibility of the $c-f$ coupling diverges) will enhance the tendency towards heavy fermi liquid order and suppress the tendency towards the spin-liquid insulating phase. This conclusion is further confirmed by the (zero temperature) phase diagram Fig. 4 obtained by explicitly solving the self-consistent equation (the boundary in this phase diagram is the same previously shown in Fig. 2(a)). As can be seen from Fig. 4, the insulating spin liquid phase has a dome shape in the phase diagram, which will be suppressed by very small or large $t_d$. The gray dashed line indicates the critical value of $V_f$, above which $E_2$ band is fully occupied and the metallic phase has a single Fermi surface. The orange dashed line marks the boundary where the two heavy fermion bands start to develop an indirect gap, which occurs for parameters above such orange line (see further discussion in Section IV).
B. Particle-hole dispersion

In this section we discuss the results for the case where itinerant electrons are hole-like which can be accounted for by simply changing $t_c \rightarrow -t_c$ in their energy dispersion (Eq. (5c)).

1. Phase-boundary

It turns out that when the metallic electron’s band structure is hole-like, the susceptibility $\chi_{cf}$ will have a stronger $\xi$ dependence compared to the particle-particle case. It can be shown that within the spin liquid phase ($V_f = 0$), that it is given by:

$$\chi_{cf}^{(0)} = \frac{2}{3\Lambda^2(t_f + t_c)} \ln\left(\frac{(T_f/t_c + \xi)(T_f/t_c + 2 - \xi)}{T_f/t_c(1 - \xi)^2}\right),$$

thus for $\xi = 1$, i.e., when both the itinerant electrons and spinons are at half-filling, the two bands are perfectly nested, the band structure leads to a divergent susceptibility $\chi_{cf}$ for all values of $t_d$, which indicates that the spin liquid phase is unstable against a transition into the Kondo insulating phase at arbitrarily small $V$. Fig. 5(a) shows the phase boundary between the insulating spin liquid and the heavy fermion metallic phase, similar to the particle-particle case, as $t_d \rightarrow 0$, the critical value of $J_K \sim V^2/U$ decreased logarithmically with $t_d$. Moreover, for the particle-hole case, the phase boundary now also has a $\xi$-dependence, as expected from the $\xi$-dependence of $\chi_{cf}^{(0)}$. As $\xi \rightarrow 1$, the spin liquid phase is suppressed and when $\xi = 1$, it only exists along the $V = 0$ line. It should be noted that at $V = 0$, the critical $t_d/U$ for the Mott transition is always the same “universal” value around $1/8$, this is because the $d$ and $e$ electrons are decoupled in this case and the problem reduces to the metal to insulator transition for the triangular lattice Hubbard model.

2. Turning on of the heavy fermion phase

For the case with $\xi < 1$, weakly inside the heavy-fermion metallic phase, where the quasi-particles’ energy dispersion $E_{1,k}$ and $E_{2,k}$ has the Mexican hat shape, it turns out that in order to maintain the half filling constraint of the spinon, we find that $E_{2,k}$ band is fully filled while the $E_{1,k}$ band is partially occupied and features two Fermi surfaces, as shown explicitly by the green dashed lines in Fig. 1(b). The $\mu_F$ can be solved from $\langle f_{i,\sigma}^\dagger f_{i,\sigma}\rangle = 1/2$ and the $\chi_{cf}$ as a function of $V_f$ can be obtained accordingly. Similar to the particle-particle case, at finite $t_d$, $\chi_{cf}$ tends to saturate as $V_f \rightarrow 0$ and it is diverging in the
atomic limit ($t_d \to 0$). For rather large $V_f$, $E_{1,\Lambda}$ becomes smaller than 0 and there is only one Fermi surface for the system (see the yellow dashed lines in Fig. 1(b)). A plot of $\chi_{cf}$ at $\xi=0.6$ is shown in Fig. 5(b), as expected, it is a decreasing function of $V_f$. The phase diagram for this case is shown in Fig. 6.

As for the special case when $\xi=1$, as explained before, because the spinon and the itinerant electron bands are nested in this case, the susceptibility $\chi_{cf}$ is diverging as $V_f \to 0$. As a result, one naturally expect a weak coupling instability from the spin liquid state to that with heavy electrons. Notice that however this state is not a metal but a Kondo insulator, since the Fermi surfaces are completely gapped out by the hybridization due to the perfect nesting. As can be seen from Fig. 7, the Kondo insulating phase turns on more rapidly for larger $t_d/U$. The phase diagram for this case is shown in Fig. 8.

IV. TUNNELLING DOS

In this section, we discuss the behaviour of the local density of states of the correlated $d$ electrons in the metallic phase which is a quantity of direct experimental relevance since it can be measured by scanning tunnelling microscopy. The thermal Green function of $d$ electron can be written as:

$$G_d(\tau, r) = -\langle T_\tau d_R^{\dagger}(r) d_R^{\dagger}(0) \rangle,$$

where $G_f(\tau, r)$ and $G_0(\tau, r)$ are Green functions of the spinon and rotor, with the definition:

$$G_f(\tau, r) = -\langle T_\tau f_R^{\dagger}(r) f_R^{\dagger}(0) \rangle,$$

$$G_0(\tau, r) = \langle T_\tau e^{i\theta_R(\tau)} e^{-i\theta_R(0)} \rangle.$$

As pointed out from previous studies [21, 24], the Matsubara Green function of $d$ electrons can be separated into a coherent part and an incoherent part:

$$G_d(\omega_n, r) = G_d^{coh}(\omega_n, r) + G_d^{inc}(\omega_n, r),$$

$$G_d^{coh}(\omega_n, r) = \Phi^2 G_f(\omega_n, r).$$

The coherent part is mainly peaked at $\omega \sim 0$ while the incoherent part captures features at larger energy scales $\omega \sim U$. In this work, we are mainly interested in the feature of LDOS near $\omega = 0$ and we will focus on the coherent part. From slave rotor mean-field theory, since the fermionic part of the Hamiltonian is non-interacting, it can be shown that the Matsubara Green function of spinon has the form:

$$G_f(\omega_n, k) = \cos^2(\alpha_k) G_1(\omega_n, k) + \sin^2(\alpha_k) G_2(\omega_n, k),$$

FIG. 5. (a) Phase boundary for particle-hole dispersion at various filling of the metallic electrons. As $\xi \to 1$, the spin liquid phase gets suppressed and at exactly half-filling of the metal, it can exist only within the $V=0$ line. (b) $\chi_{cf}$ as a function of $V_f$ for the particle-hole dispersion with $\xi=0.6$, $T_f=0.1t_d$. Similar to the particle-particle case, $\chi_{cf}$ is a decreasing function of $V_f$.

FIG. 6. Phase diagram for the particle-hole case with $\xi=0.6$. The spin liquid phase has a dome shape and the phase boundary has qualitatively the same behaviour as the particle-particle case.

FIG. 7. $\Phi$ as a function of $V^2/U$ for $\xi=1$ at different value of $t_d/U$. As expected, the metallic phase turns on in the form of a weak coupling instability with $V$. 

$$G_d^{inc}(\omega_n, r) = \Phi^2 G_f(\omega_n, r).$$

(25a)

(25b)

(26)
and the local density of state for the spinon
the Anderson limit (see Fig. 9(a)), the mean-field LDOS
gram, as indicated by the black dotted lines in Fig. 4. In
diate near the metal-insulator transition of Hubbard model.

taneously as the physics should not be very sensitive to
itinerant electrons to be
particle case and we take the bare band filling of the
be particle like, here we explored in detail the particle-
where the dispersion of itinerant electron is likely to
2e
2
2

FIG. 8. Phase diagram for the particle-hole case with \( \xi = 1 \).
The system is in Kondo insulating at any finite \( V \) since the
Fermi surface of the heavy electrons are fully gapped out, and
the spin liquid phase exists strictly only at the \( V = 0 \) line.

where \( G_{1/2}(i\omega_n, k) = 1/(i\omega_n - E_{1/2,k}) \) are the Green
function of the self-consistent band diagonal quasiparticles that result from the coherent mixing of the cor-
related and the itinerant electron. By analytical continu-
ation, the spectral function of the spinons can be easily
obtained:

\[
A_f(\omega, k) = -\frac{1}{\pi} \text{Im} G_f(\omega + i0^+, k) = \cos^2(\alpha_k)\delta(\omega - E_{1,k}) + \sin^2(\alpha_k)\delta(\omega - E_{2,k}),
\]

and the local density of state for the spinon
\( \rho_f(\omega) = \frac{1}{N} \sum_k A_f(\omega, k) \) can be obtained accordingly.

A. Zero temperature mean-field LDOS

We are particularly interested in understanding the
tunnelling density of states for experiments in 1T-TaSe2
where the dispersion of itinerant electron is likely to
be particle like, here we explored in detail the particle-
particle case and we take the bare band filling of the
itinerant electrons to be \( \xi = 1.2 \) (this value is taken ar-
borarily as the physics should not be very sensitive to
the detailed value of \( \xi \)). We are mainly focused on three
types of regime: (i) Anderson limit with \( t_d = 0 \), (ii) moder-
ate \( t_d \) along the orange dashed line in Fig. 4, (iii) large \( t_d \)
near the metal-insulator transition of Hubbard model.

Fig. 9 shows the zero temperature LDOS of corre-
lated \( d \) electrons at different regimes of the phase dia-
gram, as indicated by the black dotted lines in Fig. 4. In
the Anderson limit (see Fig. 9(a)), the mean-field LDOS
opens a coherent band gap enhanced by increasing the
Kondo coupling \( J_K \), which is the expected behaviour for
the periodic Anderson model. When \( t_d/U \) is finite (see
Figs. 9(b), (c) and (d)), the spinon acquires a band dis-

\[
B. Broadening due to finite temperature and

At finite temperature the tunneling conductance is
given by the local DOS convolved with thermal broaden-
ing due to thermal distribution of electrons in the lead.
This effect has been removed in the experiment [25] and
we also do not include it in our theory. After removing
this, it is notable that the experiment shows a single peak
which can be fitted with a Lorentzian with a temperature
dependent width:

\[
\Gamma_{exp} = \sqrt{2T^2_K + \pi^2T^2},
\]

This form of the width was found in the early experiment
that detected the Kondo peak in a single impurity case
and has been considered a signature of the single impurity
Kondo problem [25]. The low temperature width there-
fore allows to extract \( T_K \) from experiments. Further-
more, at large temperatures compared to \( T_K \) the width
scales approximately as \( \pi T \), which places a constraint
on the theory. We have re-examined the theoretical ba-

still linear in $T$ but with a coefficient which is smaller. The coefficient of the $T^2$ term in Eq. (28) is smaller by a factor of 3 in the large $N$ mean-field theory. Details are given in the Appendix B. Consequently we do not fit the experimental data to the single impurity Kondo problem, but rather to the periodic Anderson-Hubbard model we study in this paper. As we shall see below, by introducing a Fermi liquid type quasiparticle life-time together with a disorder induced width, it is possible to fit the data in certain parameter ranges.

As it is well known from the theory of single Kondo impurity and Kondo lattice problems [26-29], the fluctuations around the mean-field configuration which give rise to quasi-particle interactions, lead to a characteristic temperature and frequency dependent quasi-particle lifetime. In order to account for these effects, we add the following semi-phenomenological imaginary part to the quasi-particle self-energy [30]:

$$\Sigma_{FL}(\omega, T) = -i \frac{1}{2\pi E_0} (\omega^2 + (\pi k_B T)^2).$$

(29)

In addition to the intrinsic quasi-particle interaction effects, disorder is another important agent in broadening the density of states in experiments, and we account for this by adding a constant impurity scattering rate $\gamma_0$ into the imaginary part of the self-energy, as follows:

$$G_{1/2}(\omega + i\delta_0, k) = \frac{1}{\omega - E_{1/2,k} - \Sigma(\omega, T)}$$

$$\Sigma(\omega, T) = -i\gamma_0 + \Sigma_{FL}(\omega, T).$$

(30a)

(30b)

It should be noted that the energy scale $E_0$ controlling the quasi-particle interaction effects in Eq. (29), is usually of the order of the bandwidth for a normal Fermi liquid (large $t_d$), while for a Kondo lattice ($t_d = 0$), it is of the order of the Kondo temperature $T_K \sim 2V^2 / D_c$, with $D_c$ being the half bandwidth of itinerant electrons. In order to capture both regimes, we use a phenomenological expression of $E_0$ that interpolates between these two limits, as follows:

$$E_0 = \sqrt{T_K^2 + W_{sp}^2},$$

(31)

with $W_{sp}$ being the spinon bandwidth.

As mentioned above, in the Anderson limit, the mean-field LDOS will have two peaks separated by the gap. However, once the self-energy is included, the mean-field spectral function will be broadened and it is possible to obtain a single-peak behaviour. This can be seen clearly from Fig. 10, which shows the case of $t_d/U = 0$, $V^2/U = 0.5 t_c$ (as indicated by the $\bullet$ in Fig. 4). Even by including only the $\Sigma_{FL}$ (see Fig. 10(a)), at very low temperatures, the LDOS has two peaks separated by a band gap. When a finite impurity scattering rate (here we take $\gamma_0 = 0.05 t_c$) is taken into account, the LDOS is broadened into a single-peak behaviour, as shown in Fig. 10(b). We further calculated the half maximum half width of LDOS at different temperatures and compare it with the experimental results. We fit our theoretical data with a function of the form

$$\Gamma/t_c = \sqrt{(\Gamma_0/t_c)^2 + a\pi^2 (k_B T/t_c)^2},$$

(32)

which is expected for the single-impurity Anderson model [31, 32]. Previous theoretical works find that the experimental data can be well fitted with $a \approx 1$. According to our theoretical calculation, for the case with $V^2/U = 0.5 t_c$ and $\gamma_0 = 0.05 t_c$, the data can be well fitted with $a \approx 0.85$, as can be seen from Fig. 10(c), where all quantities are presented in unit of $t_c$. Nevertheless, once we take $t_c = 105$ meV so that the lowest temperature width matches with the experimental one, we also find quantitatively good fit to the experimental result. In other words, the experimental data can be described by a periodic Anderson model with a finite impurity scattering rate.

When $t_d$ is finite, as shown in the mean-field results above, one expects to see either a plateau-like peak (with
FIG. 10. LDOS for the particle-particle case ($\xi = 1.2$) with $t_d/U = 0, V^2/U = 0.5 t_c$ (indicated by ■ in Fig. 4). (a) LDOS with the self-energy being $\Sigma_{FL}(\omega, T)$ only. It is clear that in the low temperature limit, the spectral function has the two-peak behaviour at $\omega \sim 0$, which is due to the opening of a band gap in the mean-field energy dispersion of heavy quasiparticles. This is the signature of a coherent heavy Fermion band in the kondo lattice problem. At higher temperature, there is only a single peak around $\omega \sim 0$ due to the broadening effect from the temperature term in $\Sigma_{FL}(\omega, T)$. (b) LDOS for self-energy being as in Eq. (30a) with $\gamma_0 = 0.05 t_c$. In this case the disorder effect ($\gamma_0$ term) is able to broaden the LDOS and changes it into a single-peak behaviour. (c) and (d) shows the width of LDOS in this case. (c) Width in unit of $t_c$. (d) Fitting to experimental data with $t_c = 105$ meV. The experimental data can be well fitted by the theoretical result.

small $J_K$) or a finite gap sandwiched by two peaks (rather large $J_K$) in the LDOS. In any case, the inclusion of a finite imaginary self-energy can broaden the curve. Along the orange line, since the two mean-field bands of heavy quasiparticles are about to separate, the LDOS of spinon should have only a single peak around $\omega \sim 0$. Figs. 11 and 12 show two points close to the line: $t_d/U = 0.04$, $V^2/U = 0.35 t_c$, and $t_d/U = 0.08$, $V^2/U = 0.65 t_c$, (indicated by • and ◇ respectively in Fig. 4), it is clear that the LDOS has only a single peak at $\omega \sim 0$. As for the width, we find that the width as a function of temperature can also be relatively well fitted by Eq. (32). To compare with the experimental data, as we did for the Anderson limit, one can tune $t_c$ such that the lowest temperature limit of the width is consistent with the experimental one. Fig. 11(c) and Fig. 12(c) show the comparison of the width between the theoretical and experimental results. $t_c$ is taken to be 120 meV and 75 meV separately. We can see that the small spinon hopping case $t_d = 0.04 t_c$ can give rise to a good fit to the experimental data. For the larger $t_d$ case ($t_d/U = 0.08$) the fit deteriorates because the coefficient $\alpha$ is becoming too small.

We also checked cases with moderate $t_d/U$ but being farther away from the orange dashed line: $t_d/U = 0.04$, $V^2/U = 0.8$ and $t_d/U = 0.08$, $V^2/U = 0.3$ (indicated by ◊ and ● respectively in Fig. 4). Figs. 13 (a) and (b) show the LDOS for the first case without and with $\gamma_0$ included in the self-energy, and the LDOS for the latter case (without and with $\gamma_0$ in the self-energy) are presented in Figs. 14(a) and (b). The first case is above the orange dashed line in Fig. 4 with a large $J_K$, and the two quasiparticle bands are separated in energy. So the LDOS (Fig. 13(a)) has a gap sandwiched by two peaks. In the later case, which is below the orange dashed line, the two quasiparticle bands overlap with each other and there is a flat peak in LDOS (see Fig. 14(a)). Once
FIG. 12. LDOS at $t_d/U = 0.08$, $V^2/U = 0.65 t_c$ (indicated by $\star$ in Fig. 4). (a)-(b) LDOS without/with $\gamma_0$ in the self-energy. (c) Fitting of the width to experiment with $t_c = 75$ meV. In this case the theory lies below the data because the slope $\alpha$ is becoming too small.

FIG. 13. LDOS at $t_d/U = 0.04$, $V^2/U = 0.8 t_c$ (indicated by $\bullet$ in Fig. 4). (a)-(b) LDOS without/with impurity scattering in the self-energy. (c) Fitting of the width to experiment with $t_c = 60$ meV. This case is much above the orange dashed line in Fig. 4 and the two quasiparticle bands are separated form each other.

FIG. 14. LDOS at $t_d/U = 0.08$, $V^2/U = 0.3 t_c$ (indicated by $\bullet$ in Fig. 4). (a)-(b) LDOS without/with impurity scattering in the self-energy. (c) Fitting of the width to experiment with $t_c = 110$ meV. This case is below the orange dashed line and the two quasiparticle bands overlaps. $\gamma_0$ is introduced for both cases, the LDOS changes into a single peak behaviour for both cases (Fig. 13(b) and Fig. 14(b)). The fitting of LDOS width to the experimental data for these two cases are shown in Fig. 13(c) and Fig. 14(c). One can see that while the parameter $a$ for $t_d/U = 0.04$ still gives a reasonable fit, the value of $a$ for $t_d/U = 0.08$, $V^2/U = 0.3$ is too small and the width cannot be well fitted by Eq. (32). We conclude that as $t_d/U$ increases, the fit deteriorates, especially away from the orange dashed line.

Finally, for large $t_d/U$ (here we take $t_d/U = 0.11$) close to the critical value for the metal-insulator transition in the isolated Hubbard model, the LDOS for $V^2/U = 0.1 t_c$ and $V^2/U = 0.3 t_c$ (indicated by $\bigtriangleup$ and $\Delta$ separately in Fig. 4) are shown in Fig. 15 and Fig. 16. As expected, the LDOS has a flat top near $\omega = 0$ without the inclusion of $\gamma_0$ in the self-energy (Fig. 15(a) and Fig. 16(a)), and will be broadened once $\gamma_0$ is introduced (Fig. 15(b) and Fig. 16(b)). Fig. 15(c) and Fig. 16(c) show the width for these cases and we see that the experimental data cannot be fitted by the theoretical results in this regime because the theoretical slope is too small. To summarize, by including a Fermi liquid type of (imaginary) self-energy into heavy quasiparticles’ Green function, it is possible to obtain a single-peak behaviour for the LDOS even in the Anderson limit. By modifying the value of $\gamma_0$, the width of LDOS can be well fitted by Eq. (32), which is the formula for a single impurity Kondo problem. Moreover, adjusting $t_c$ to fit the experimental width value at
the lowest temperature, our theory suggests that the experimental situation may be in or close to the Anderson limit of the model. On the other hand, for intermediate \( t_d/U \) a reasonable fit can be obtained when the Kondo scale \( J_K \) and the Heisenberg scale \( J_H \) compete, resulting in a low temperature width which is smaller than \( J_K \) or \( J_H \). In addition, our theory predicts \( a \sim 0.3 \) if the hopping of the \( d \) electrons is close to the critical value of for the metal-insulator transition in isolated Hubbard model, a value which does not fit the experimental data.

V. SUMMARY AND DISCUSSIONS

We have studied a model of coupled correlated and itinerant electrons which naturally interpolates between the periodic Anderson model and the Hubbard model. Using a slave rotor mean-field approach we have obtained a phase diagram that summarizes the competition between a spinon fermi surface state weakly coupled to a metal and an interlayer coherent heavy fermi liquid metallic state (illustrated in Figs. 4, 5 and 7). In the localized or atomic limit where our model reduces to the periodic Anderson model, the Kondo coupling needed to destroy the spin liquid in favor of the metal, \( J_K \sim V^2/U \), has a logarithmic dependence on the hopping of the correlated electrons in the putative spin liquid layer \( t_d/U \), reflecting that the emergent scales determining the competition are the Kondo temperature \( T_K \sim e^{-1/J_K} \) and Heisenberg coupling \( J_H \sim t_d^2/U \). Therefore although technically in such limit the spin liquid is destabilized via a weak coupling instability, the critical Kondo coupling, \( J_K \), needed to destabilize the spin liquid grows rather fast with the Heisenberg coupling, giving rise to the rapid rise of the boundary between the spin liquid and the heavy metal at small \( t_d/U \) seen in Figs. 4, 5 and 7. In this limit one can use the measured saturation width \( T_K \) to place an upper bound on the Heisenberg coupling \( J_H \), resulting in a rather small bound of about 5 meV from the experiments of Ref. [17]. On the other hand, at larger values of \( t_d/U \sim 0.1 \) when the spin liquid has a sizable bandwidth, the critical \( J_K \) is comparable to \( t_d/U \), and near the Mott transition the critical Kondo coupling needed to destabilize the spin liquid vanishes linearly with the distance of \( t_d/U \) away from the critical value associated with the Mott metal-insulator-transition, at mean field level. However, we find that generically the peak width is dominated by the spinon bandwidth, leading to a width that is too broad and with too weak a temperature dependence to explain the data. The exception is when the system happens to fall near the crossover line indicated in orange in Fig. 4, where a reasonable fit to the data can also be obtained. In this case, the Kondo scale \( J_K \) and the Heisenberg scale \( J_H \) compete, giving rise to a narrow peak with a width which is smaller than either scale at low temperature. As a result, in this case the low
temperature width cannot be used as a bound for either scale, and it is possible that $J_H$ is much larger than the 5 meV bound mentioned previously.

The above conclusion was reached by studying the LDOS of the heavy metal throughout this phase diagram, which can be directly accessed via STM experiments [17]. In the local moment periodic Anderson limit of the model the coherent hybridization of correlated and itinerant electrons in the heavy metal leads to the bare LDOS acquiring a two-peak structure due to the opening of a direct optical band gap. On the other hand near the Mott-metal-insulator transition the LDOS features a rather flat shape due to a relatively large spinon band width. The measured LDOS is however further broadened by the intrinsic lifetime of the heavy quasi-particles arising from their interactions and also by disorder, leading to a smearing of the double-peak structure in the periodic Anderson model limit. We have argued that including these effects renders the double peak structure effectively into a single peak, and we have found good agreement with the shape and temperature dependence of the peak reported in recent STM experiments [17]. We also find reasonable fit to the data at intermediate $t_d/U$ in the vicinity of the orange line in Fig. 4.

We note that in the localized limit of small $t_d/U$ the Hubbard model in the triangular lattice is expected not to form a spinon Fermi surface state, but to order into a conventional 120° AFM phase. This piece of physics is not captured in our slave rotor mean-field theory, which favors spin disordered ground states. Therefore, our results pose a challenge for the interpretation of the behavior of the stand-alone putative 1T-TaSe$_2$ as a quantum spin liquid: if indeed the system is near the Anderson limit, this raises the possibility that it could be instead comprised of localized moments that are rather weakly coupled and might ultimately weakly order at yet lower temperatures in cleaner samples. However we caution that we cannot definitely rule out that the putative spin liquid layer is at an intermediate coupling strength $t_d/U$ that brings the system closer to the Mott transition, where also a small interlayer tunnelling can destabilize the spin liquid. An additional consideration is that the actual 1T-TaSe$_2$ system involves multiple bands and is probably not described by a single band Mott-Hubbard model. While the spin liquid is stabilized only near the Mott transition in a single band model [22], it is possible that a multi-band description can extend the spin liquid to lower effective $t_d$.

Additionally, to re-iterate the potential uncertainties, we wish to note that the parameter $a$ in Eq. (32) that we used near the Mott transition has a Fermi liquid form but it can be changed by tuning the value of $\gamma_0$ and $E_0$, which are respectively controlled by disorder and quasiparticle interactions, and hence are inherently difficult scales to estimate accurately.

We want also to point out that in our calculation, we considered the metallic electrons to have the same lattice constant and Brillouin zone as the correlated electrons. In doing so, we are imagining that in a more microscopic description one would be folding the Brillouin of the metallic 1H-TaSe$_2$, which does match with the smaller Brillouin zone of the star of David structure of 1T-TaSe$_2$, and that after this one is only including one of the folded bands of itinerant electrons. However, the hybridization with electrons at higher energy scales (coming from other folded bands) could also play an important role in determining the phase boundary and the form of LDOS, but such details lie beyond the scope of the considerations that we have explored in the present work.

ACKNOWLEDGMENTS

We thank Michael F. Crommie, Wei Ruan and Yi Chen for sharing their data and discussions. We also thank Peng Rao for fruitful discussions. PAL acknowledges support by DOE office of Basic Sciences grant number DE-FG02-03-ER46076.

Appendix A: Finite Temperature Rotor Mean Field Approach

As mentioned in the main text, for the order parameter of metallic phase, $\Phi = \langle e^{i\theta} \rangle$, we estimate its value by taking the average with respect to a single site Hamiltonian:

$$H^{(1)}_\theta = -K_\theta (e^{i\theta} + e^{-i\theta}) + \frac{U}{2} n_\theta^2$$

$$= H_K + H_U,$$

where $H_K = -K_\theta (e^{i\theta} + e^{-i\theta})$ and $H_U = \frac{U}{2} n_\theta^2$. We have taken $\lambda = 0$ to fulfill the constrain Eq. (3) and the half-filling of the spinon. Because we are interested in the large $U$ limit of the model ($t_d/U = 1/8$), it is reasonable to use a first-order perturbation (in $H_K$) to estimate the expectation value:

$$\langle e^{i\theta} \rangle = \frac{\text{Tr} (e^{-\beta H_K} e^{i\theta} e^{\beta H_U})}{\text{Tr} (e^{-\beta (H_K + H_U)})}$$

$$= \sum \int_0^\beta d\tau \langle e^{-\beta H_U} e^{\tau H_K} e^{-\tau H_U} e^{i\theta} \rangle / \text{Tr} (e^{-\beta H_U}),$$

one can take the trace with the eigenbasis of angular momentum $\eta_\theta$: $\{|n\rangle\}$, which satisfies: $n_\theta |m\rangle = m |m\rangle$ and $e^{i\theta} |n\rangle = |n + 1\rangle$, and we will denote the eigenvalue of $H_U$ by $E_n = \frac{U}{2} n^2$. It is straightforward to obtain:

$$- \int_0^\beta d\tau \text{Tr} (e^{-\beta H_U} e^{\tau H_K} e^{-\tau H_U} e^{i\theta})$$

$$= K_\theta \sum_n \int_0^\beta d\tau e^{-\beta E_n} e^{-\beta E_n} e^{i(E_n - E_{n+1})}$$

$$= K_\theta \sum_n \frac{e^{-\beta E_{n+1}} - e^{-\beta E_n}}{E_n - E_{n+1}},$$

$$= \frac{U}{2}$$
so one finally arrives at:

\[ \langle e^{i\theta} \rangle \approx \chi_{\theta,1} K_\theta, \]  

(A5)

\[ \chi_{\theta,1} = \sum_n \frac{e^{-\beta E_{n+1}} - e^{-\beta E_n}}{E_n - E_{n+1}} \approx \sum_n e^{-\beta E_n}. \]  

(A6)

By Taking the zero temperature limit, one can recover the zero temperature result given by:

\[ \lim_{\beta \to \infty} \chi_{\theta,1}(\beta) = 4/U. \]  

(A7)

Next, we extrapolate the expression above, which is valid only for small \( K_\theta \), with the phenomenological formula:

\[ \langle e^{i\theta} \rangle = \frac{K_\theta}{\sqrt{\chi_{\theta,1}^2 + K_\theta^2}}, \]  

(A8)

which recovers the behavior from Eq. (A5) at small \( K_\theta \) and also the approach of \( \langle e^{i\theta} \rangle \to 1 \), which is expected at large \( K_\theta \) (and it is also consistent with the constraint that \( \langle e^{i\theta} \rangle \leq 1 \)).

For \( \langle e^{-i\theta}, e^{i\theta} \rangle \), one can perform same kind of calculation. We estimate it by taking the expectation value with respect to the Hamiltonian:

\[ \tilde{H}_\theta = \frac{U}{2} \sum_i n_{\delta,i}^2 - 2T_\theta \sum_{\langle i,j \rangle} \left( e^{-i\theta} e^{i\theta_j} + h.c. \right), \]  

(A9)

taking \( T_\theta \)-term as a perturbation, after some algebra, one obtains that:

\[ \langle e^{-i\theta} e^{i\theta_j} \rangle = \chi_{\theta,2} T_\theta, \]  

(A10)

\[ \chi_{\theta,2} = 2 \left( \sum_{n,n+1} e^{-\beta(E_{n+1} - E_n)} - e^{-\beta(E_n + E_{n+1})} \right) \]  

\[ + \sum_n \beta e^{-\beta(E_n + E_{n+1})} \left( \sum_n e^{-\beta E_n} \right)^2, \]  

(A11)

and for the zero temperature limit, one recovers the value \( \chi_{\theta,2} \approx 4/U \). Because we are interested in small \( t_d \) limit (remember that \( T_\theta = t_d \chi(0) \)), we simply use Eq. (A10) throughout our calculations.

**Appendix B: Tunnelling DOS of the single impurity Anderson Model**

In this section, we briefly review the theory of tunnelling DOS for a single impurity Anderson model and comment on the fitting of STM results in previous studies by Nagaoka et al. [25].

For a single impurity Anderson model, one can calculate the tunnelling DOS of the local electron using perturbation theory since there is no phase transition as the on-site interaction \( U \) increases [20]. Early theoretical calculations [31, 32] shows that the (retarded) Green function of the local electron for the particle-hole symmetric case reads (valid at small \( \omega \) and \( T \)):

\[ G_d(\omega, T) = \frac{1}{\omega - \epsilon_d - \text{Re} \Sigma(\omega) + i\Delta - i \text{Im} \Sigma(\omega, T)} \]  

(B1)

with

\[ Z = \frac{1}{1 - \partial_\omega \text{Re} \Sigma(\omega)|_{\omega=0}}, \]  

(B2a)

\[ \tilde{\epsilon}_d = Z (\epsilon_d + \text{Re} \Sigma(0)) \approx 0, \]  

(B2b)

\[ \text{Im} \Sigma(\omega, T) = \frac{\Delta}{2} \left( \frac{\omega}{T_K} \right)^2 + \frac{\epsilon_d^2}{T_K}. \]  

(B2c)

In the previous work by Nagaoka et al. [25], \( \text{Re} \Sigma(\omega) \) in Eq. (B1) was replaced by \( -\epsilon_d \) and the first term in the denominator \( \omega \) was dropped, based on the argument that it is \( T_K/\Delta \) smaller than \( \text{Im} \Sigma(\omega, T) \). However, the more standard procedure is to expand \( \text{Re} \Sigma(\omega) \) around the pole, leading to a term \( (\omega - \epsilon_d)/Z \) in the denominator, which leads to the second line in Eq. (B1). This term is the same order as \( \text{Im} \Sigma(\omega, T) \) and must be kept. Then it is straightforward to obtain the spectral function:

\[ \rho_d(\omega) = \frac{Z}{\omega^2 + Z^2 (\Delta + \text{Im} \Sigma(\omega))^2} \]  

(B3)

\[ = \frac{\Delta^2}{2} \frac{1}{\omega^2 + \frac{e^2}{16\pi T_K^2}(1 + \frac{2}{\pi^2} (\omega^2 + \frac{\epsilon_d^2}{T_K^2}))^2}, \]  

in small \( \omega \) and low temperature limit, to the lowest order of \( \omega/T_K \) and \( T/T_K \), the spectral function can be approximated as:

\[ \rho_d(\omega) \approx \frac{1}{\pi \Delta} \frac{1}{\left( \frac{\pi^2}{4\pi T_K} \right)^2 + \frac{1}{3\pi^2} \omega^2 + \frac{\epsilon_d^2}{3\pi^2 T_K^2}}, \]  

(B4)

which has a Lorentzian form and the half maximum width is:

\[ \Gamma_{\text{theory}} = \sqrt{\frac{32}{3\pi^2} T_K + \frac{1}{3} \frac{\omega^2}{\pi^2 T^2}}. \]  

(B5)

As mentioned earlier, in Nagaoka et al. [25], the quasi-particle spectral weight factor \( Z \) was neglected and the \( \omega^2 \) term in the denominator of Eq. (B3) was dropped, and it was found that

\[ \rho_d(\omega, T) = \frac{1}{\pi \Delta} \frac{1}{1 + \left( \frac{\omega}{\sqrt{2} T_K} \right)^2} \frac{1}{1 + \frac{\epsilon_d^2}{2T_K^2}}, \]  

(B6)

thus leading to the width of the form:

\[ \Gamma_{\text{exp}} = \sqrt{2 T_K^2 + \pi^2 T^2}, \]  

(B7)
Compared with Eq. (B5), the discrepancy in the first term inside the square root can be absorbed by a redefinition of $T_K$, but one can see that there is a discrepancy in the coefficient before the $\pi^2 T^2$ term which is directly measurable. We note that the precise coefficient in Eq. (B5) depends on the mean-field theory, and the coefficient in Eq. (B7) is an upper-bound. It is interesting that the experimental data can be fitted so well by the formula Eq. (B7), which was obtained “improperly” from theoretical result. This might be due to some other effects in the experiments, such as disorder scattering effects.

[1] P. W. Anderson, Science 235, 1196 (1987).
[2] C. Broholm, R. J. Cava, S. A. Kivelson, D. G. Nocera, M. R. Norman, and T. Senthil, Science 367, eaay0668 (2020).
[3] L. Savary and L. Balents, Rep. Prog. Phys. 80, 016502 (2016).
[4] Y. Zhou, K. Kanoda, and T.-K. Ng, Rev. Mod. Phys. 89, 025003 (2017).
[5] K. T. Law and P. A. Lee, Proc. Natl. Acad. Sci. U.S.A. 114, 6996 (2017).
[6] W.-Y. He, X. Y. Xu, G. Chen, K. Law, and P. A. Lee, Phys. Rev. Lett. 121, 046401 (2018).
[7] K. Rossnagel, J. Phys. Condens. Matter 23, 213001 (2011).
[8] M. Kratochvilova, A. D. Hillier, A. R. Wildes, L. Wang, S.-W. Cheong, and J.-G. Park, npj Quantum Materials 2, 42 (2017).
[9] M. Klanjšek, A. Zorko, R. Žitko, J. Mravlje, Z. Jagličič, P. K. Biswas, P. Prelovšek, D. Mihailovic, and D. Arčon, Nat. Phys. 13, 1130 (2017).
[10] J. Wilson, F. D. Salvo, and S. Mahajan, Adv. Phys. 24, 117 (1975).
[11] A. Ribak, I. Silber, C. Baines, K. Chashka, Z. Salman, Y. Dagan, and A. Kanigel, Phys. Rev. B 96, 195131 (2017).
[12] Y. J. Yu, Y. Xu, L. P. He, M. Kratochvilova, Y. Y. Huang, J. M. Ni, L. Wang, S.-W. Cheong, J.-G. Park, and S. Y. Li, Phys. Rev. B 96, 081111 (2017).
[13] H. Murayama, Y. Sato, T. Taniguchi, R. Kurihara, X. Z. Xing, W. Huang, S. Kasahara, Y. Kasahara, I. Kimchi, M. Yoshida, Y. Iwasa, Y. Mizukami, T. Shibuchi, M. Konczykowski, and Y. Matsuda, Phys. Rev. Research 2, 013099 (2020).
[14] K. Rossnagel and N. V. Smith, Phys. Rev. B 73, 073106 (2006).
[15] F. Di Salvo, R. Maines, J. Waszczak, and R. Schwall, Solid State Commun. 14, 497 (1974).
[16] Y. Chen, W. Ruan, M. Wu, S. Tang, H. Ryu, H.-Z. Tsai, R. Lee, S. Kahn, F. Liou, C. Jia, O. R. Albertini, H. Xiong, T. Jia, Z. Liu, J. A. Sobota, A. Y. Liu, J. E. Moore, Z.-X. Shen, S. G. Louie, S.-K. Mo, and M. F. Crommie, Nat. Phys. 16, 218 (2020).
[17] W. Ruan, Y. Chen, S. Tang, J. Hwang, H.-Z. Tsai, R. Lee, M. Wu, H. Ryu, S. Kahn, C. Jia, A. Aikawa, C. Hwang, F. Wang, Y. Choi, S.-G. Louie, P. A. Lee, Z.-X. Shen, S.-K. Mo, and M. F. Crommie, arXiv e-prints, arXiv:2009.07379 (2020), arXiv:2009.07379 [cond-mat.str-el].
[18] S. Doniach, Physica B+C 91, 231 (1977).
[19] A. C. Hewson, The Kondo Problem to Heavy Fermions, Cambridge Studies in Magnetism (Cambridge University Press, 1993).
[20] P. Coleman, Introduction to Many-Body Physics (Cambridge University Press, 2015).
[21] S. Florens and A. Georges, Phys. Rev. B 70, 035114 (2004).
[22] S.-S. Lee and P. A. Lee, Phys. Rev. Lett. 95, 036403 (2005).
[23] O. I. Motrunich, Phys. Rev. B 72, 045105 (2005).
[24] E. Zhao and A. Paramekanti, Phys. Rev. B 76, 195101 (2007).
[25] K. Nagaoka, T. Jainneala, M. Grobis, and M. F. Crommie, Phys. Rev. Lett. 88, 4 (2002).
[26] N. Read and D. M. Newns, J. Phys. Condens. Matter 16, 3273 (1983).
[27] N. Read and D. M. Newns, J. Phys. Condens. Matter 16, L1055 (1983).
[28] P. Coleman, Phys. Rev. B 29, 3035 (1984).
[29] A. Auerbach and K. Levin, Phys. Rev. B 34, 3524 (1986).
[30] L. Zheng and S. D. Sarma, Phys. Rev. B 53, 9964 (1996).
[31] K. Yamada, Prog. Theor. Exp. Phys. 53, 970 (1975).
[32] T. A. Costi, A. C. Hewson, and V. Zlatic, J. Phys. Condens. Matter 6, 2519 (1994), 9310032.