

Fermi surface enlargement on the Kondo lattice

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The Kondo lattice model is a paradigmatic model for the description of local moment systems, a class of materials exhibiting a range of strongly correlated phenomena including heavy fermion formation, magnetism, quantum criticality, and unconventional superconductivity. Conventional theoretical approaches invoke fractionalization of the local moment spin through large- N and slave particle methods. In this work we develop a formalism based on noncanonical degrees of freedom, building upon a recently developed approach for strongly correlated electrons [E. Quinn, *Phys. Rev. B* **97**, 115134 (2018)]. Specifically, we demonstrate that higher dimensional representations of $su(2|2)$ correspond to a splitting of the electronic degree of freedom on the Kondo lattice, in a manner which entwines the conduction electrons with the local moment spins. This provides a powerful means of organizing correlations, and offers a perspective on heavy fermion formation. Unlike slave-particle methods, noncanonical degrees of freedom generically allow for a violation of the Luttinger sum rule, and we interpret recent angle resolved photoemission experiments on Ce-115 systems in view of this.

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I. INTRODUCTION

Metals with local moments provide a rich playground to study unconventional phases and quantum phase transitions. A range of interesting phenomena, including unconventional superconductivity and non-Fermi liquid behavior, arise from competition between magnetism and the Kondo effect [1–5]. When magnetism wins and the local moments order, the electrons are free to form a canonical Fermi liquid. When the Kondo effect dominates, the local moment is quenched by the conduction electrons, giving rise to “heavy” electronic quasiparticles with effective masses as large as $1000m_e$ [6]. This heavy fermion state is also characterized by an enlargement of the Fermi surface, observed in Hall conductivity [7,8], magnetostriction [9], quantum oscillation [10], and angle resolved photoemission (ARPES) [11–15] experiments. These two regimes are generally separated by critical behavior associated with Kondo breakdown, which manifests itself as a non-Fermi liquid fan extending to finite temperatures [16–21].

A precise estimation of the enlargement of the Fermi volume \mathcal{V}_{FS} requires a complete mapping of the Fermi surface, a challenging task only very recently achieved with ARPES [13–15]. The conclusions are remarkable: CeCoIn₅ [13], CeIrIn₅ [14], and CeRhIn₅ [15] all show enlargement which is significantly smaller than the anticipated $\mathcal{V}_{FS} \propto n_c + n_f$, where n_c and n_f are the conduction electron and local moment densities, respectively. For instance, in CeCoIn₅ [13] the enhancement is only $\mathcal{V}_{FS} \propto n_c + 0.2 \pm 0.05$.

These observations suggest a violation of Luttinger’s sum rule, a direct proportionality between electron density and Fermi surface volume which has been established for a canonical Fermi liquid [22–24].

Although the Kondo impurity problem is exactly solvable [25–27], there is no exact solution for the Kondo lattice model. The standard analytic approaches such as large- N employ fractionalization of the local moment spin [18,28,29]. Within this approach there are two possibilities for the Fermi surface volume: (i) $\mathcal{V}_{FS} \propto n_c$ when there is no Kondo hybridization which occurs at high temperature; (ii) $\mathcal{V}_{FS} \propto n_c + n_f$ once the Kondo hybridization sets in. This enlargement of the Fermi surface is attributed to the local moment spin becoming delocalized, thereby gaining charge in relation to Luttinger’s sum rule. Dynamical mean-field theory [30,31], which is exact in infinite dimensions, goes beyond the large- N mean-field description by introducing finite lifetime effects, but is in qualitative agreement with respect to Luttinger’s sum rule.

It is worth highlighting that these systems are not the only cases where evidence for the violation of Luttinger’s sum rule is observed. Another prominent example is the pseudogap regime of the cuprates, where quantum oscillation and Hall and thermal conductivity experiments indicate the existence of a Fermi surface whose volume drops to zero as half-filling is approached [32–34]. The analogy can be strengthened by drawing a parallel between the non-Fermi liquid behavior appearing between the small and large Fermi surface regimes in local moment systems with that occurring between the Fermi liquid and pseudogap regimes in the cuprates [35]. Linking rearrangement of the Fermi surface and non-Fermi liquid behavior offers a promising paradigm for characterizing the phase diagram of strongly correlated electronic matter.

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In this article we develop a theoretical framework for local moment systems. We demonstrate that the degrees of freedom of local moment systems can be reinterpreted through the noncanonical graded Lie algebra $su(2|2)$, and exploit this to obtain a systematic description of strongly correlated behavior. The resulting regime can be interpreted as a splitting of the electronic degree of freedom [36], and exhibits a self-hybridization of the band structure inducing a heavy effective mass and enlargement of the Fermi surface.

The formalism we employ violates Luttinger's sum rule quite generally. Central to Luttinger's theorem is the organization of the correlations of an interacting system around canonical fermion degrees of freedom via the Schwinger-Dyson equation, let us cast it as $\mathcal{G} = \frac{1}{g_0^{-1} - \Sigma}$. Recently it has been established that correlations can instead be organized around noncanonical degrees of freedom via an exact representation of the Green's function as $\mathcal{G} = g\Omega = \frac{\Omega}{g_0^{-1} - \Sigma}$, where Ω encodes the correlations resulting from the noncanonical nature of the degree of freedom [37,38]. In the purely electronic setting it was shown that this generically yields a violation of Luttinger's sum rule [36]. This can be regarded as formalizing Hubbard's approach based on graded projection operators [39,40], as well as providing a framework for systematically going beyond it. Here we obtain a nontrivial generalization to the local moment setting, where the connection to graded projection operators is lost, but the splitting of the electron is maintained, giving rise again to violation of Luttinger's sum rule.

II. LOCAL MOMENT SYSTEMS

We consider the Kondo lattice Hamiltonian

$$H = \sum_{p,\sigma} (\varepsilon_p - \mu) c_{p\sigma}^\dagger c_{p\sigma} + J_K \sum_i \vec{s}_i \cdot \vec{S}_i, \quad (1)$$

an archetypal model to describe local moment physics in which itinerant electrons interact with local spin moments at each site of the lattice through a Kondo coupling. Here \vec{s} denotes the conduction electron spin

$$s^z = \frac{1}{2}(\mathbf{n}_\uparrow - \mathbf{n}_\downarrow), \quad s^+ = c_\uparrow^\dagger c_\downarrow, \quad s^- = c_\downarrow^\dagger c_\uparrow, \quad (2)$$

and \vec{S} denotes local moment spin. We consider the general case of a spin- S local moment, and so the Hilbert space at each site is $4(2S+1)$ dimensional. For example, for the case of a spin-1/2 local moment there are eight states per site: $|\downarrow\rangle, c_\downarrow^\dagger |\downarrow\rangle, c_\uparrow^\dagger |\downarrow\rangle, c_\downarrow^\dagger c_\uparrow^\dagger |\downarrow\rangle, |\uparrow\rangle, c_\downarrow^\dagger |\uparrow\rangle, c_\uparrow^\dagger |\uparrow\rangle, c_\downarrow^\dagger c_\uparrow^\dagger |\uparrow\rangle$.

In the absence of the Kondo coupling, when $J_K = 0$, the electrons and local moments are decoupled. For $J_K \neq 0$ however the interaction induces correlations in the system, and our objective is to identify those which allow for a good effective description of the resulting behavior. Heuristically, we wish to identify the relevant degrees of freedom, and organize the correlations about these. In practice, a quantum degree of freedom is specified by the algebra it obeys and this algebra provides the mathematical structure for organizing the correlations induced by the interacting Hamiltonian.

Let us outline two distinct ways of characterizing the local degree of freedom. First, the standard way is to regard the electrons and spin moments independently.

Here the electrons are governed by the canonical anticommutation relations $\{c_\sigma, c_{\sigma'}^\dagger\} = \delta_{\sigma\sigma'}$, and the local spin moments are governed by the $su(2)$ algebra $[S^z, S^\pm] = \pm S^\pm$, $[S^+, S^-] = 2S^z$. These provide reasonable degrees of freedom for a regime of behavior where the electrons form a Fermi liquid with a "small" Fermi surface and the spins are free to order at low temperatures, as seen for example in CeRh_2Si_2 [41].

In this article we pursue a distinct description of the local degree of freedom. This builds upon recent work arguing that the graded Lie algebra $su(2|2)$ is a valid degree of freedom for organizing correlations in the purely electronic setting [36]. The $su(2|2)$ algebra admits a family of $4(2S+1)$ -dimensional representations [42,43], which have a natural interpretation as combining a local spin moment with the electron. Let us consider fermionic operators written explicitly in terms of c and S as follows:

$$\begin{aligned} q_{\downarrow\circ}^\dagger &= \frac{1}{2}c_\uparrow + \frac{\lambda}{2S+1} \left(\frac{1}{2}c_\uparrow - \mathbf{n}_\downarrow c_\uparrow + c_\downarrow S^- + c_\uparrow S^z \right), \\ q_{\uparrow\circ}^\dagger &= \frac{1}{2}c_\downarrow + \frac{\lambda}{2S+1} \left(\frac{1}{2}c_\downarrow - \mathbf{n}_\uparrow c_\downarrow + c_\uparrow S^+ - c_\downarrow S^z \right), \\ q_{\downarrow\bullet}^\dagger &= \frac{1}{2}c_\downarrow^\dagger - \frac{\lambda}{2S+1} \left(\frac{1}{2}c_\downarrow^\dagger - \mathbf{n}_\uparrow c_\downarrow^\dagger + c_\uparrow^\dagger S^- - c_\downarrow^\dagger S^z \right), \\ q_{\uparrow\bullet}^\dagger &= -\frac{1}{2}c_\uparrow^\dagger + \frac{\lambda}{2S+1} \left(\frac{1}{2}c_\uparrow^\dagger - \mathbf{n}_\downarrow c_\uparrow^\dagger + c_\downarrow^\dagger S^+ + c_\uparrow^\dagger S^z \right). \end{aligned} \quad (3)$$

These are related back to the canonical fermion operators through

$$c_\downarrow^\dagger = q_{\uparrow\circ} + q_{\downarrow\bullet}^\dagger, \quad c_\uparrow^\dagger = q_{\downarrow\circ} - q_{\uparrow\bullet}^\dagger, \quad (4)$$

and so we refer to this as a splitting of the electron, as in the electronic case.

Let us examine the algebra they generate. First, the anticommutation relations of the q are

$$\begin{aligned} \{q_{\sigma\nu}, q_{\sigma\nu}^\dagger\} &= \frac{1+\lambda^2}{4} + \frac{\lambda}{2S+1} (\nu\eta^z - \sigma\Sigma^z), \\ \{q_{\downarrow\nu}, q_{\uparrow\nu}^\dagger\} &= \frac{\lambda}{2S+1} \Sigma^+, \quad \{q_{\sigma\circ}, q_{\sigma\bullet}^\dagger\} = \frac{\lambda}{2S+1} \eta^+, \\ \{q_{\uparrow\nu}, q_{\downarrow\nu}^\dagger\} &= \frac{\lambda}{2S+1} \Sigma^-, \quad \{q_{\sigma\bullet}, q_{\sigma\circ}^\dagger\} = \frac{\lambda}{2S+1} \eta^-, \\ \{q_{\sigma\nu}, q_{\sigma'\nu'}\} &= \{q_{\sigma\nu}^\dagger, q_{\sigma'\nu'}^\dagger\} = \frac{1-\lambda^2}{4} \epsilon_{\sigma'\sigma} \epsilon_{\nu\nu'}, \end{aligned} \quad (5)$$

which generate the total spin operators

$$\vec{\Sigma} = \vec{s} + \vec{S}, \quad (6)$$

combining the electronic and local moment spin, and the electronic charge operators

$$\eta^z = \frac{1}{2}(\mathbf{n}_\uparrow + \mathbf{n}_\downarrow - 1), \quad \eta^+ = c_\downarrow^\dagger c_\uparrow^\dagger, \quad \eta^- = c_\uparrow c_\downarrow. \quad (7)$$

In evaluating these anticommutators the Casimir identity $\vec{S} \cdot \vec{S} = S(S+1)$ is used. The commutation relations between the q and Σ are

$$\begin{aligned} [\Sigma^z, q_{\uparrow\nu}^\dagger] &= \frac{\sigma}{2} q_{\uparrow\nu}^\dagger, \quad [\Sigma^z, q_{\sigma\nu}] = -\frac{\sigma}{2} q_{\sigma\nu}, \\ [\Sigma^+, q_{\downarrow\nu}^\dagger] &= -q_{\uparrow\nu}^\dagger, \quad [\Sigma^+, q_{\uparrow\nu}] = q_{\downarrow\nu}, \\ [\Sigma^-, q_{\uparrow\nu}^\dagger] &= -q_{\downarrow\nu}^\dagger, \quad [\Sigma^-, q_{\downarrow\nu}] = q_{\uparrow\nu}, \end{aligned} \quad (8)$$

and between the \mathbf{q} and $\boldsymbol{\eta}$ are

$$\begin{aligned} [\eta^z, \mathbf{q}_{\sigma\nu}^\dagger] &= \frac{\nu}{2} \mathbf{q}_{\sigma\nu}^\dagger, & [\eta^z, \mathbf{q}_{\sigma\nu}] &= -\frac{\nu}{2} \mathbf{q}_{\sigma\nu}, \\ [\eta^+, \mathbf{q}_{\sigma\circ}^\dagger] &= \mathbf{q}_{\sigma\bullet}^\dagger, & [\eta^+, \mathbf{q}_{\sigma\bullet}] &= -\mathbf{q}_{\sigma\circ}, \\ [\eta^-, \mathbf{q}_{\sigma\bullet}^\dagger] &= \mathbf{q}_{\sigma\circ}^\dagger, & [\eta^-, \mathbf{q}_{\sigma\circ}] &= -\mathbf{q}_{\sigma\bullet}. \end{aligned} \quad (9)$$

The $\boldsymbol{\Sigma}$ and $\boldsymbol{\eta}$ mutually commute, and each obeys an $su(2)$ algebra

$$\begin{aligned} [\boldsymbol{\Sigma}^z, \boldsymbol{\Sigma}^\pm] &= \pm \boldsymbol{\Sigma}^\pm, & [\boldsymbol{\Sigma}^+, \boldsymbol{\Sigma}^-] &= 2\boldsymbol{\Sigma}^z, \\ [\eta^z, \eta^\pm] &= \pm \eta^\pm, & [\eta^+, \eta^-] &= 2\eta^z. \end{aligned} \quad (10)$$

In this way the \mathbf{q} generate the $su(2|2)$ algebra whose algebraic relations are Eqs. (5) and (8)–(10). Furthermore, the algebra is extended to $u(2|2)$ by incorporating the generator

$$\boldsymbol{\theta} = \frac{1}{2} - \frac{1}{2S+1} \left(\vec{\Sigma} \cdot \vec{\Sigma} + \frac{1}{3} \vec{\eta} \cdot \vec{\eta} \right), \quad (11)$$

which obeys

$$\begin{aligned} [\boldsymbol{\theta}, \mathbf{q}_{\sigma\nu}^\dagger] &= \frac{1+\lambda^2}{4\lambda} \mathbf{q}_{\sigma\nu}^\dagger + \frac{1-\lambda^2}{4\lambda} \epsilon_{\sigma\sigma'} \epsilon_{\nu\nu'} \mathbf{q}_{\sigma'\nu'}, \\ [\boldsymbol{\theta}, \mathbf{q}_{\sigma\nu}] &= -\frac{1+\lambda^2}{4\lambda} \mathbf{q}_{\sigma\nu} - \frac{1-\lambda^2}{4\lambda} \epsilon_{\sigma\sigma'} \epsilon_{\nu\nu'} \mathbf{q}_{\sigma'\nu'}, \end{aligned} \quad (12)$$

and commutes with the $\boldsymbol{\Sigma}$ and $\boldsymbol{\eta}$.

The set of generators

$$8 \times \mathbf{q}, \quad 3 \times \mathbf{s}, \quad 3 \times \boldsymbol{\eta}, \quad \boldsymbol{\theta} \quad (13)$$

thus offer a second way to characterize the local degree of freedom on the Kondo lattice. Our intention now is to regard these as composite operators, and to employ the algebra they obey to organize correlations so as to gain access to a strongly correlated regime of behavior. Their algebra is noncanonical, for example, the anticommutation relations of the \mathbf{q} yield the generators of the spin and charge $su(2)$ subalgebras. This obstructs the use of canonical methods for evaluating two-point functions of the \mathbf{q} . The noncanonical terms, however, come with a prefactor $\frac{\lambda}{2S+1}$, and we will employ a formalism recently introduced by Shastry to organize the correlations they induce. A powerful consequence of the splitting of the electron, Eq. (4), is that once the two-point functions of the \mathbf{q} are obtained then the electronic Green's function follows immediately through linear combinations.

To proceed, it is necessary to reexpress the Kondo lattice model through the generators (13). The kinetic term becomes quadratic in \mathbf{q} , through the linearity of Eq. (4). The Kondo interaction $\vec{s} \cdot \vec{S}$ can be reexpressed as quadratic in $\boldsymbol{\Sigma}$ and quartic in \mathbf{q} , as both \mathbf{s} and \mathbf{S} give terms quadratic in \mathbf{q} through Eqs. (2) and (6). It is, however, also possible to reexpress the Kondo interaction in a simpler way. For this we rewrite Eq. (11) using the operator identities $\vec{s} \cdot \vec{s} = \frac{3}{4}(\mathbf{n}_\uparrow - \mathbf{n}_\downarrow)^2$, $\vec{\eta} \cdot \vec{\eta} = \frac{3}{4}(\mathbf{n}_\uparrow + \mathbf{n}_\downarrow - 1)^2$, $\vec{s} \cdot \vec{s} + \vec{\eta} \cdot \vec{\eta} = \frac{3}{4}$, and $\vec{S} \cdot \vec{S} = S(S+1)$ to obtain

$$\vec{s} \cdot \vec{S} = \frac{1}{3} \vec{\eta} \cdot \vec{\eta} - \frac{2S+1}{2} \boldsymbol{\theta} - \frac{1+4S^2}{8}. \quad (14)$$

This convenient expression reflects the power of recasting the Kondo lattice model through $su(2|2)$. It allows us to cleanly identify the role of the Kondo coupling in splitting

the electronic band, due to linear action of $\boldsymbol{\theta}$ on \mathbf{q} from Eq. (12).

III. ORGANIZING STRONG CORRELATIONS

We now exploit the $su(2|2)$ algebra to gain access to a strongly correlated regime of behavior. Let us emphasize that we do not require the algebra $su(2|2)$ to provide an explicit symmetry of the model in any way; instead we use it to organize correlations. Our ultimate objective is to compute the electronic Green's function

$$\mathcal{G}_{ij\sigma}^{\text{el}}(\tau) = -\langle \mathbf{c}_{i\sigma}(\tau) \mathbf{c}_{j\sigma}^\dagger(0) \rangle = -\frac{1}{\mathcal{Z}} \text{Tr}(e^{-\beta H} \mathcal{T}[\mathbf{c}_{i\sigma}(\tau) \mathbf{c}_{j\sigma}^\dagger(0)]), \quad (15)$$

where $\mathcal{Z} = \text{Tr} e^{-\beta H}$, β is inverse temperature, $\mathbf{a}(\tau) = e^{\tau H} \mathbf{a} e^{-\tau H}$, and \mathcal{T} is the τ -ordering operator which is antisymmetric under interchange of fermionic operators.

This section closely mirrors Sec. III of Ref. [36] and we adopt similar notations for the reader's convenience. To simplify, we collect the fermionic generators as

$$\boldsymbol{\psi}_i^\alpha = (\mathbf{q}_{i\uparrow\circ}^\dagger \quad \mathbf{q}_{i\downarrow\bullet} \quad \mathbf{q}_{i\downarrow\circ}^\dagger \quad \mathbf{q}_{i\uparrow\bullet} \quad \mathbf{q}_{i\uparrow\circ} \quad \mathbf{q}_{i\downarrow\bullet}^\dagger \quad \mathbf{q}_{i\downarrow\circ} \quad \mathbf{q}_{i\uparrow\bullet}^\dagger), \quad (16)$$

with Greek indices, and the bosonic generators as

$$\boldsymbol{\phi}_i^a = (\boldsymbol{\Sigma}_i^z \quad \boldsymbol{\Sigma}_i^- \quad \boldsymbol{\Sigma}_i^+ \quad \eta_i^z \quad \eta_i^- \quad \eta_i^+), \quad (17)$$

with Latin indices. The $u(2|2)$ algebra is then compactly expressed as

$$\begin{aligned} \{\boldsymbol{\psi}_i^\alpha, \boldsymbol{\psi}_j^\beta\} &= \delta_{ij} (f^{\alpha\beta} \mathbf{I} + f^{\alpha\beta} \mathbf{a} \boldsymbol{\phi}_i^a), \\ [\boldsymbol{\phi}_i^a, \boldsymbol{\psi}_j^\beta] &= \delta_{ij} f^{\alpha\beta} \boldsymbol{\psi}_i^\gamma, \quad [\boldsymbol{\phi}_i^a, \boldsymbol{\phi}_j^b] = \delta_{ij} f^{ab} \boldsymbol{\phi}_i^c, \\ [\boldsymbol{\theta}_i, \boldsymbol{\psi}_j^\alpha] &= \delta_{ij} f^{\Theta\alpha} \boldsymbol{\psi}_i^\beta, \quad [\boldsymbol{\theta}_i, \boldsymbol{\phi}_j^a] = 0, \end{aligned} \quad (18)$$

where summation over repeated algebraic indices is implied. Explicit expression for the structure constants f can be read from Eqs. (5) and (8)–(10), and given explicitly in the Appendix.

The Kondo lattice Hamiltonian can then be re-expressed in terms of the split-electron degrees of freedom

$$\mathbf{H} = -\sum_{(i,j)} t_{ij,\alpha\beta} \boldsymbol{\psi}_i^\alpha \boldsymbol{\psi}_j^\beta + \sum_i V_{ab} \boldsymbol{\phi}_i^a \boldsymbol{\phi}_i^b + \sum_i V_\Theta \boldsymbol{\theta}_i - \mu_a \sum_i \boldsymbol{\phi}_i^a. \quad (19)$$

Here $\langle i, j \rangle$ denotes the summation is over pairs of sites, and the nonzero hopping parameters are $t_{ij,51} = t_{ij,61} = t_{ij,52} = t_{ij,62} = t_{ij,73} = -t_{ij,83} = -t_{ij,74} = t_{ij,84} = t_{ij}$ and their antisymmetric pairs $t_{ij,\alpha\beta} = -t_{ij,\beta\alpha}$, where $t_{ij} = -\frac{1}{\mathcal{V}} \sum_p e^{ip(i-j)} \varepsilon_p$ with \mathcal{V} the total number of lattice sites. The remaining nonzero parameters are $V_{44} = 2V_{56} = 2V_{65} = \frac{1}{3} J_K$, $V_\Theta = -\frac{2S+1}{2} J_K$, and $\mu_4 = 2\mu$.

We set ourselves the intermediate objective of computing the matrix Green's function of the \mathbf{q} , that is

$$\mathcal{G}_{ij\beta}^\alpha(\tau, \tau') = -\langle \boldsymbol{\psi}_i^\alpha(\tau) \boldsymbol{\psi}_{j\beta}(\tau') \rangle, \quad (20)$$

where $\boldsymbol{\psi}_{i\alpha} = (\boldsymbol{\psi}_i^\alpha)^\dagger = \boldsymbol{\psi}_i^\beta K_{\beta\alpha}$, which defines K given explicitly in the Appendix. The electronic Green's function

is immediately obtained from linear combinations of these,

$$\begin{aligned} \mathcal{G}_{ij\downarrow}^{\text{el}}(\tau) &= \mathcal{G}_{ij1}^1(\tau) + \mathcal{G}_{ij2}^1(\tau) + \mathcal{G}_{ij1}^2(\tau) + \mathcal{G}_{ij2}^2(\tau), \\ \mathcal{G}_{ij\uparrow}^{\text{el}}(\tau) &= \mathcal{G}_{ij3}^3(\tau) - \mathcal{G}_{ij4}^3(\tau) - \mathcal{G}_{ij3}^4(\tau) + \mathcal{G}_{ij4}^4(\tau), \end{aligned} \quad (21)$$

via Eqs. (4).

The challenge in computing \mathcal{G} is the noncanonical nature of the algebraic relations Eq. (18), which obstructs the use of Wick's theorem. To proceed we follow Shastry [37,38] and employ the Schwinger formalism, introducing sources for the bosonic generators ϕ into the imaginary-time thermal expectation value as follows:

$$\langle \mathcal{O}(\tau) \rangle = \frac{\text{Tr}(e^{-\beta H} \mathcal{T}[e^{\int_0^\beta d\tau' S(\tau')} \mathcal{O}(\tau)])}{\text{Tr}(e^{-\beta H} \mathcal{T}[e^{\int_0^\beta d\tau' S(\tau')}]}, \quad (22)$$

with $S(\tau) = \sum_i \zeta_{ia}(\tau) \phi_i^a(\tau)$. Then bosonic correlations can be traded for functional derivatives through

$$\langle \phi_i^a(\tau) \mathcal{O}(\tau') \rangle = (\langle \phi_i^a(\tau) \rangle + \nabla_i^a(\tau)) \langle \mathcal{O}(\tau') \rangle, \quad (23)$$

where $\nabla_i^a(\tau) = \frac{\delta}{\delta \zeta_{ia}(\tau^+)}$, and $\tau^+ = \tau + 0^+$ incorporates an infinitesimal regulator which ensures a consistent ordering when $\tau = \tau'$.

The matrix Green's function obeys the equation of motion

$$\begin{aligned} \partial_\tau \mathcal{G}_{ij\beta}^\alpha(\tau, \tau') &= -\delta(\tau - \tau') \{ \psi_i^\alpha(\tau), \psi_{j\beta}(\tau) \} \\ &+ \langle [\mathcal{S}(\tau), \psi_i^\alpha(\tau)] \psi_{j\beta}(\tau') \rangle \\ &- \langle [\mathbf{H}, \psi_i^\alpha(\tau)] \psi_{j\beta}(\tau') \rangle, \end{aligned} \quad (24)$$

together with the antiperiodic boundary condition $\mathcal{G}_{ij\beta}^\alpha(\beta, \tau') = -\mathcal{G}_{ij\beta}^\alpha(0, \tau')$. Evaluating the algebraic relations, it takes the form

$$\begin{aligned} \sum_k [\delta_{ik} (-\delta_\gamma^\alpha \partial_\tau - f^{a\alpha}{}_\gamma \zeta_{ia}(\tau) - \mu_a f^{a\alpha}{}_\gamma + V_\Theta f^{\Theta\alpha}{}_\gamma - f^{a\alpha}{}_\delta V_{ab} f^{b\delta}{}_\gamma + 2f^{a\alpha}{}_\gamma V_{ab} (\langle \phi_i^b(\tau) \rangle + \nabla_i^b(\tau))) \\ + f^{\alpha\delta}{}_l t_{ik,\delta\gamma} + f^{\alpha\delta}{}_a t_{ik,\delta\gamma} (\langle \phi_i^a(\tau) \rangle + \nabla_i^a(\tau))] \mathcal{G}_{kj\beta}^\gamma(\tau, \tau') \\ = \delta(\tau - \tau') \delta_{ij} (f^{\alpha\gamma}{}_l + f^{\alpha\gamma}{}_a \langle \phi_i^a(\tau) \rangle) K_{\gamma\beta}. \end{aligned} \quad (25)$$

The canonical way to proceed here is to invert \mathcal{G} via the Schwinger-Dyson equation, but this is obstructed by the nontrivial expectation value on the right-hand side. Here we bypass this difficulty by adopting Shastry's trick of factorizing \mathcal{G} in two:

$$\mathcal{G}_{ij\beta}^\alpha(\tau, \tau') = \sum_l \int_0^\beta d\tau'' \mathfrak{g}_{il\gamma}^\alpha(\tau, \tau'') \Omega_{lj\beta}^\gamma(\tau'', \tau'). \quad (26)$$

Distributing the functional derivative in Eq. (25) across these factors, and bringing the terms with the functional derivative acting on Ω to the right-hand side, a simplification can be made by exploiting the arbitrariness in the definition of Ω to set

$$\Omega_{ij\beta}^\alpha(\tau, \tau') = \delta(\tau - \tau') \delta_{ij} (f^{\alpha\gamma}{}_l + f^{\alpha\gamma}{}_a \langle \phi_i^a(\tau) \rangle) K_{\gamma\beta} - \sum_{k,l} \int_0^\beta d\tau'' (f^{\alpha\epsilon}{}_a t_{il,\epsilon\delta} + 2\delta_{il} f^{b\alpha}{}_\delta V_{ba}) \mathfrak{g}_{lk\gamma}^\delta(\tau, \tau'') \nabla_i^a(\tau) \Omega_{kj\beta}^\gamma(\tau'', \tau'). \quad (27)$$

The equation of motion then reduces to

$$\begin{aligned} \sum_k [\delta_{ik} (-\delta_\gamma^\alpha \partial_\tau - f^{a\alpha}{}_\gamma \zeta_{ia}(\tau) - \mu_a f^{a\alpha}{}_\gamma + V_\Theta f^{\Theta\alpha}{}_\gamma - f^{a\alpha}{}_\delta V_{ab} f^{b\delta}{}_\gamma + 2f^{a\alpha}{}_\gamma V_{ab} (\langle \phi_i^b(\tau) \rangle + \nabla_i^b(\tau))) \\ + f^{\alpha\delta}{}_l t_{ik,\delta\gamma} + f^{\alpha\delta}{}_a t_{ik,\delta\gamma} (\langle \phi_i^a(\tau) \rangle + \nabla_i^a(\tau))] \mathfrak{g}_{kj\beta}^\gamma(\tau, \tau') = \delta(\tau - \tau') \delta_{ij}. \end{aligned} \quad (28)$$

We have thus converted Eq. (25) with one unknown \mathcal{G} into two equations, (27) and (28), with two unknowns Ω , \mathfrak{g} . The advantage is that Eq. (27) is a closed functional equation for Ω , while Eq. (28) has the form of a canonical equation of motion, and thus can be inverted through the Schwinger-Dyson equation in the standard way as follows:

$$\mathfrak{g}_{ij\beta}^{-1\alpha}(\tau, \tau') = \mathfrak{g}_{0,ij\beta}^{-1\alpha}(\tau, \tau') - \Sigma_{ij\beta}^\alpha(\tau, \tau'), \quad (29)$$

where \mathfrak{g}_0 is given exactly through

$$[\delta_{ik} (-\delta_\gamma^\alpha \partial_\tau - f^{a\alpha}{}_\gamma \zeta_{ia}(\tau) - \mu_a f^{a\alpha}{}_\gamma + V_\Theta f^{\Theta\alpha}{}_\gamma) + f^{\alpha\delta}{}_l t_{ik,\delta\gamma}] \mathfrak{g}_{0,kj\beta}^\gamma(\tau, \tau') = \delta(\tau - \tau') \delta_{ij} \delta_\beta^\alpha, \quad (30)$$

and Σ obeys the closed functional equation

$$\begin{aligned} \Sigma_{ij\beta}^\alpha(\tau, \tau') &= \delta(\tau - \tau') \delta_{ij} f^{a\alpha}{}_\gamma V_{ab} f^{b\gamma}{}_\beta - \delta(\tau - \tau') (f^{\alpha\gamma}{}_a t_{ij,\gamma\beta} + 2\delta_{ij} f^{b\alpha}{}_\beta V_{ba}) \langle \phi_i^a(\tau) \rangle \\ &- \delta(\tau - \tau') \delta_{ij} \sum_l (f^{\alpha\epsilon}{}_a t_{il,\epsilon\delta} + 2\delta_{il} f^{b\alpha}{}_\delta V_{ba}) \mathfrak{g}_{li\gamma}^\delta(\tau, \tau^+) f^{a\gamma}{}_\beta \\ &- \sum_{k,l} \int_0^\beta d\tau'' (f^{\alpha\epsilon}{}_a t_{il,\epsilon\delta} + 2\delta_{il} f^{b\alpha}{}_\delta V_{ba}) \mathfrak{g}_{lk\gamma}^\delta(\tau, \tau'') \nabla_i^a(\tau) \Sigma_{kj\beta}^\gamma(\tau'', \tau'). \end{aligned} \quad (31)$$

In this way, we obtain an exact representation of \mathcal{G} through Eqs. (26), (27), (29)–(31) via an exact rewriting of the equation of motion for \mathcal{G} . While at first sight these expressions may appear complicated, conceptually they are quite simple. Schematically the Green's function of the \mathbf{q} is cast in the form $\mathcal{G} \sim \mathfrak{g}\Omega \sim \frac{\Omega}{\mathfrak{g}_0^{-1} - \Sigma}$, where \mathfrak{g}_0^{-1} is known exactly and both Ω and Σ obey exact closed functional equations. The appearance of a nontrivial numerator here is intuitively understood as capturing the correlations resulting from the noncanonical nature of the degree of freedom.

In general we cannot solve these equations exactly, i.e., we cannot gain complete control of all correlations in the system. Instead we use them to organize the correlations: Ω and Σ can be computed through a perturbative expansion in $\frac{\lambda}{2S+1}$ and J_K , under the principle that the leading contributions capture the crucial correlations governing the behavior in the regime governed by these noncanonical degrees of freedom. In the following section we focus on the simplest nontrivial approximation, which is to suppress the terms containing functional derivatives in Eqs. (27) and (31). This is the static approximation, the analog of Hartree-Fock for a canonical degree of freedom, where both Ω and Σ are frequency independent.

We conclude by highlighting a subtlety arising in the local moment setting which is absent in the purely electronic case, i.e., for $S = 0$. This concerns computing terms of the form $\langle \phi \rangle$ and $\nabla \langle \phi \rangle$. In the electronic case the ϕ are quadratic in ψ , and so $\langle \phi \rangle$ is directly obtained from \mathcal{G} . For $S \neq 0$, however, it is not quite this simple. The spin generators are $\tilde{\mathbf{S}} = \vec{s} + \vec{S}$, and while \vec{s} is quadratic in \mathbf{q} , it is necessary to understand how to handle the contributions of the form $\langle S \rangle$ and $\nabla \langle S \rangle$. In the following we focus on the normal state within an approximation for which this subtlety does not affect the analysis.

IV. STATIC APPROXIMATION

We proceed to study the static approximation to the Green's function resulting from an organization of the correlations around the split-electron $su(2|2)$ degrees of freedom. This amounts to neglecting the functional derivative terms in Eqs. (27) and (31), which are suppressed in $\frac{\lambda}{2S+1}$ and J_K . We focus on the normal state, and so the only possible nonzero $\langle \phi_i(\tau) \rangle$ is $\langle \eta_i^z(\tau) \rangle = \varphi_\beta^\alpha \mathcal{G}_{ii\alpha}^\beta(\tau, \tau^+)$, with φ given explicitly in the Appendix.

We thus set the sources to zero and switch to Fourier space according to

$$\mathcal{G}_{p\sigma}(i\omega_n) = \frac{1}{\mathcal{V}} \sum_{i,j} \int_0^\beta d\tau e^{i\omega_n\tau - ip(i-j)} \mathcal{G}_{ij\sigma}(\tau), \quad (32)$$

with Matsubara frequencies $\omega_n = (2n+1)\frac{\pi}{\beta}$, $n \in \mathbb{Z}$, and \mathcal{V} is the total number of lattice sites. Then Eqs. (26), (27), (29)–(31) take the closed form

$$\begin{aligned} \mathcal{G}_{p\beta}^\alpha(i\omega_n) &= \mathfrak{g}_{p\gamma}^\alpha(i\omega_n) \Omega_{p\beta}^\gamma, \\ \Omega_{p\beta}^\alpha &= (f^{\alpha\gamma}{}_I + f^{\alpha\gamma}{}_a \langle \phi^a \rangle) K_{\gamma\beta}, \\ \mathfrak{g}_p^{-1\alpha}(i\omega_n) &= \mathfrak{g}_{0,p\beta}^{-1\alpha}(i\omega_n) - \Sigma_{p\beta}^\alpha, \end{aligned}$$

$$\begin{aligned} \mathfrak{g}_{0,p\beta}^{-1\alpha}(i\omega_n) &= i\omega_n \delta_\beta^\alpha - \mu_a f^{\alpha\alpha}{}_\beta + V_\Theta f^{\Theta\alpha}{}_\beta + f^{\alpha\delta}{}_I t_{p,\delta\beta}, \\ \Sigma_{p\beta}^\alpha &= f^{\alpha\gamma}{}_\gamma V_{ab} f^{b\gamma}{}_\beta - (f^{\alpha\gamma}{}_a t_{p,\gamma\beta} + 2f^{b\alpha}{}_\beta V_{ba}) \langle \phi^a \rangle \\ &\quad - \frac{1}{\mathcal{V}} \sum_q (f^{\alpha\epsilon}{}_a t_{q,\epsilon\delta} + 2f^{b\alpha}{}_\delta V_{ba}) \tilde{\mathfrak{g}}_{q\gamma}^\delta f^{\alpha\gamma}{}_\beta, \quad (33) \end{aligned}$$

where here the nontrivial $\langle \phi^a \rangle$ is given by $\langle \eta^z \rangle = \frac{1}{\mathcal{V}} \sum_{q,m} e^{i\omega_m 0^+} \varphi_\beta^\alpha \mathcal{G}_{q\alpha}^\beta(i\omega_m)$ and $\tilde{\mathfrak{g}}_{q\beta}^\alpha = \frac{1}{\beta} \sum_m e^{i\omega_m 0^+} \mathfrak{g}_{q\beta}^\alpha(i\omega_m)$. The corresponding approximate electronic Green's function follows through Eq. (21).

To illustrate the formalism we consider the Kondo lattice model on a two-dimensional square lattice with nearest-neighbor hopping. We solve Eqs. (33) self-consistently, and focus on $J_K = 0.3$, $S = 1/2$, and zero temperature. In Fig. 1(a) we plot the electronic spectral function $A_{p\sigma}^{\text{el}} = -\frac{1}{\pi} \text{Im} \mathcal{G}_{p\sigma}^{\text{el}}(\omega + i0^+)$, which reveals the formation of heavy bands with large effective masses in the vicinity of half-filling. Unlike large- N theories, the hybridization does not follow the chemical potential as one moves away from half-filling, though this may be a limitation of the static approximation. Our band structure also does not display any noteworthy temperature dependence. Figure 1(b) displays both the direct Δ_d and the indirect Δ_{ind} gaps as a function of J_K for $\mu = 0$. Similar to large- N calculations [4], we find the two gaps are related as $\Delta_{\text{ind}} = \Delta_d^2/W$, where W is the bandwidth. Generically we find that the enlargement of the Fermi surface violates Luttinger's sum rule and this is illustrated in Fig. 1(c). While for low electron density n_c the Fermi surface volume closely obeys $V_{FS} \propto n_c$, as half-filling is approached the volume grows rapidly to $V_{FS} \propto n_c + 1$.

These results are independent of the value of λ chosen, which reflects an independence of the model parameters of Eq. (19) on λ . Specifically, this owes to a subtle cancellation between the λ dependence of Σ and Ω with the λ dependence of the uncorrelated \mathfrak{g}_0^{-1} through the structure constants $f^{\Theta\alpha}{}_\beta$ and $f^{\alpha\beta}{}_I$. Thus it seems reasonable to adopt arbitrarily small λ , supporting the noncanonical formalism we employ. It will be interesting to examine this in more detail when going beyond the static approximation. We anticipate that nontrivial λ dependence will arise if the kinetic term of the Hamiltonian takes a correlated hopping form [36].

V. SUMMARY AND DISCUSSION

In this article we have adapted a recently developed framework for characterizing strong correlations to the Kondo lattice. We have shown how the local degree of freedom can be recast through the generators of the Lie algebra $su(2|2)$ for general representations Eq. (3), corresponding to a splitting of the electron Eq. (4), and we have related the Kondo interaction to the local emergent generator θ , Eq. (14). To handle the noncanonical nature of the algebra we utilized Shastry's Green's function factorization technique, which leads to an exact representation of the \mathbf{q} Green's function, with correlations encoded through two functional equations (27) and (31), which provides systematic access to the electronic Green's function through Eq. (21).

To examine the behavior governed by these degrees of freedom we have focused on the ‘‘static’’ approximation. This

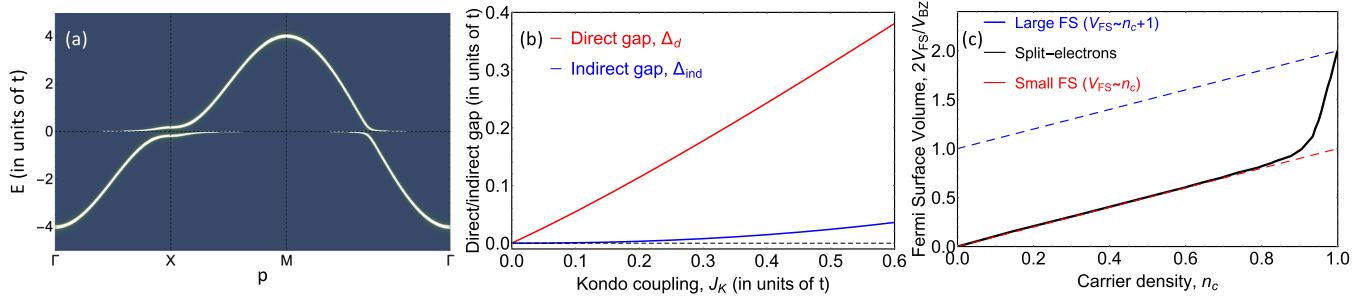


FIG. 1. Results from the static approximation within the split-electron formalism for a square lattice and $S = 1/2$: (a) intensity plot of the electronic spectral function for $J_K/t = 0.3$ and $\mu = 0$ (with Lorentzian broadening) showing the formation of heavy bands around half-filling. (b) The direct and indirect gaps as a function of J_K , which are related by $\Delta_{ind} = \Delta_d^2/W$ as in the large- N mean-field approximation [4]. (c) Violation of Luttinger’s sum rule. In contrast to standard theories where the Fermi surface volume is either $V_{FS} \propto n_c$ or $V_{FS} \propto n_c + n_f$, we find $n_c \leq \frac{2V_{FS}}{V_{BZ}} \leq n_c + 1$, where V_{BZ} is the volume of the Brillouin zone.

is a first order approximation, the analog of Hartree-Fock for a canonical degree of freedom, in which the quasiparticles are sharply defined as shown in Fig. 1(a). As a function of parameters, it is possible to have a Kondo insulator at half filling or a heavy Fermi liquid with large Fermi surface and heavy quasiparticles away from half-filling. We thus see that this captures the basic phenomenology of heavy fermions.

In contrast with prominent theories of heavy fermion formation, our analysis does not invoke a “delocalization” of the local moment spin. We find this an attractive aspect of our formalism, as the effective Kondo lattice setting has the charge of the local moment frozen out to begin with. Instead the moment’s spin is entwined with the conduction electrons into the $\mathbf{q}_{\sigma v}$, as in Eq. (3). The Kondo splitting of the electronic band arises from a hybridization between the two flavors $\mathbf{q}_{\sigma \circ}$ and $\mathbf{q}_{\sigma \bullet}$. The enlargement of the Fermi surface emerges naturally, and can be attributed to violation of Luttinger’s sum rule due to the noncanonical nature of the degrees of freedom.

Indeed, violation of the Luttinger sum rule is another attractive feature of our formalism, unambiguously distinguishing it from existing theoretical approaches. It accounts for recent ARPES studies which find that the enlargement of the Fermi surface in CeCoIn₅ [13], CeIrIn₅ [14], and CeRhIn₅ [15] is significantly smaller than the volume $V_{FS} \propto n_c + n_f$ corresponding to delocalized spin moments. Within the large- N framework, a possible explanation would be that some of the f electrons remain localized in a spin liquid. There is, however, no direct evidence for such behavior in these compounds. For instance, a putative $U(1)$ spin liquid would lead to a spinon continuum in neutron scattering experiments, and this has not been observed. In contrast, the split-electron degrees of freedom form a sharp Fermi surface and therefore recover Fermi liquid phenomenology including $\rho \sim T^2$ resistivity at low temperatures.

There are many directions for future research. Of particular importance is going beyond the static approximation considered here. For the single impurity case, we do not expect to capture Kondo resonance formation within the static approximation, in line with the conventional perspective [44]. This motivates the development of improved approximative schemes along the lines of T -matrix or RPA methods. Indeed, it is remarkable that the static approximation captures

the hybridization gap. Recent ARPES experiments [13,45] show that the temperature at which the hybridization gap starts to open can be much higher than the Kondo coherence temperature, and we anticipate that improved approximations can recover the Kondo resonance and shed light on this dichotomy.

Another direction is to address magnetism. Within the large- N framework this is a significant challenge, and attempts in this direction have been to extend the theory to supersymmetric versions [46–50]. On the other hand, although there are subtleties to be addressed within our formalism regarding magnetism, we do not expect an inherent bottleneck. It would be interesting to examine magnetism in an underscreened Kondo model, where $S > 1/2$, for instance, in the context of uranium based ferromagnets [51–53].

We conclude with a general comment, mirroring a similar analysis in the purely electronic setting [36]. We have identified two distinct ways to characterize the local degree of freedom on the Kondo lattice, either in the traditional way through the canonical fermion and local spin algebras or through the $su(2|2)$ algebra as developed here. Neither provides an exact solution of the model away from $J_K = 0$. Instead they offer two distinct quasiparticle frameworks for organizing the correlations induced by interactions. It would be interesting to explore to what extent the competition between the two sets of degrees of freedom is responsible for the non-Fermi liquid behavior associated with Kondo destruction.

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APPENDIX: COMPACT NOTATIONS

The structure constants for the representation of the $u(2|2)$ algebra in Eq. (18) are conveniently expressed through tensor

products of Pauli matrices $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. First, $f^{\alpha\beta}_I$ and $f^{\Theta\alpha}_\beta$ depend on λ as follows:

$$\begin{aligned} f^{\alpha\beta}_I &= \frac{1+\lambda^2}{4}\sigma_1 \otimes \sigma_0 \otimes \sigma_0 + \frac{1-\lambda^2}{4}\sigma_1 \otimes \sigma_3 \otimes \sigma_1, \\ f^{\Theta\alpha}_\beta &= \frac{1\pm\lambda^2}{4\lambda}\sigma_3 \otimes \sigma_0 \otimes \sigma_3 + \frac{1\pm\lambda^2}{4i\lambda}\sigma_3 \otimes \sigma_3 \otimes \sigma_2. \end{aligned} \quad (\text{A1})$$

The structure constants $f^{\alpha\beta}_a$ are proportional to $\frac{\lambda}{2S+1}$ as follows:

$$\begin{aligned} f^{\alpha\beta}_1 &= -\frac{\lambda}{2S+1}\sigma_1 \otimes \sigma_3 \otimes \sigma_3, \\ f^{\alpha\beta}_2 &= \frac{\lambda}{2S+1}\frac{\sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2}{2} \otimes \sigma_0, \\ f^{\alpha\beta}_3 &= \frac{\lambda}{2S+1}\frac{\sigma_1 \otimes \sigma_1 - \sigma_2 \otimes \sigma_2}{2} \otimes \sigma_0, \\ f^{\alpha\beta}_4 &= -\frac{\lambda}{2S+1}\sigma_1 \otimes \sigma_0 \otimes \sigma_3, \end{aligned}$$

$$\begin{aligned} f^{\alpha\beta}_5 &= \frac{\lambda}{2S+1}\frac{\sigma_0 + \sigma_3}{2} \otimes \sigma_1 \otimes \sigma_1, \\ f^{\alpha\beta}_6 &= \frac{\lambda}{2S+1}\frac{\sigma_0 - \sigma_3}{2} \otimes \sigma_1 \otimes \sigma_1. \end{aligned} \quad (\text{A2})$$

The structure constants $f^{\alpha\beta}_a$ are independent of λ as follows:

$$\begin{aligned} f^{1\alpha}_\beta &= \frac{1}{2}\sigma_3 \otimes \sigma_3 \otimes \sigma_0, \\ f^{2\alpha}_\beta &= -\frac{\sigma_3 \otimes \sigma_1 + i\sigma_0 \otimes \sigma_2}{2} \otimes \sigma_3, \\ f^{3\alpha}_\beta &= -\frac{\sigma_3 \otimes \sigma_1 - i\sigma_0 \otimes \sigma_2}{2} \otimes \sigma_3, \\ f^{4\alpha}_\beta &= -\frac{1}{2}\sigma_3 \otimes \sigma_0 \otimes \sigma_0, \\ f^{5\alpha}_\beta &= -\frac{\sigma_2 + i\sigma_1}{2} \otimes \sigma_1 \otimes \sigma_2, \\ f^{6\alpha}_\beta &= -\frac{\sigma_2 - i\sigma_1}{2} \otimes \sigma_1 \otimes \sigma_2. \end{aligned} \quad (\text{A3})$$

Also $K^\alpha_\beta = \sigma_1 \otimes \sigma_0 \otimes \sigma_0$ and $\varphi^\alpha_\beta = \frac{\sigma_3 \otimes \sigma_3 - \sigma_0 \otimes \sigma_0}{4} \otimes \sigma_1 + \frac{\sigma_3 \otimes \sigma_0 - \sigma_0 \otimes \sigma_3}{4} \otimes \sigma_0$.

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