

Solution to a Quantum Impurity Model for Moiré Systems: Fermi Liquid, Pairing, and Pseudogap

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Recent theoretical and experimental studies have revealed the co-existence of heavy and light electrons in magic-angle multilayer graphene, which form a periodic lattice of Anderson impurities hybridizing with Dirac semi-metals. This work demonstrates that nontrivial features—pairing potential [1], pseudogap [2], and continuous quantum phase transitions—already appear at the single-impurity level, if valley-anisotropic anti-Hund’s interactions (J_S, J_D) are included, favoring either a singlet ($J_S > J_D$) or a valley doublet ($J_D > J_S$) impurity configuration. We derive a complete phase diagram and *analytically* solve the impurity problem at several fixed points using bosonization and refermionization techniques. When $J_D > J_S$ and $J_D > 0$, the valley doublet only couples via pair-hopping processes to the conduction electrons, in sharp contrast to the conventional Kondo scenario. Upon increasing J_D , there is a quantum phase transition of the BKT universality class, from a Fermi liquid to an anisotropic doublet phase, the latter exhibiting power-law susceptibilities with non-universal exponents. On the other hand, when $J_S > J_D$ and $J_S > 0$, increasing J_S induces a second-order phase transition from Fermi liquid to a local singlet phase, which involves a non-Fermi liquid as an intermediate fixed point. Near the transition towards the anisotropic doublet (local singlet) phase, the renormalized interaction of the Fermi liquid becomes attractive, favoring doublet (singlet) pairing. Based on analytic solutions, we construct *ansätze* for the impurity spectral function and correlation self-energy, which account for the pseudogap accompanying side peaks, found in recent spectroscopic measurements and a DMFT study [2]. In particular, we obtain a non-analytic V-shaped spectral function with non-universal exponents in the anisotropic doublet phase. All the results are further verified by numerical renormalization group calculations.

Introduction—Moiré hetero-structures have opened up a new stage to engineer electronic flat bands, providing thrilling new possibilities to study exotic correlations besides conventional materials [3–5]. In a variety of systems, flat bands originate from the formation of local orbitals at the moiré length scale [6–9], akin to the atomic d or f shells. Compared to atomic shells, moiré orbitals can possess richer inner degrees of freedom such as layer and valley. More importantly, with an underlying lattice, electrons interact not only through the Coulomb repulsion, but also through microscopic processes such as phonons [10, 11], which act non-trivially on the new degrees of freedom. These aspects imply that, even for a model as simple as a local orbital, new physics is yet to be explored.

One paradigmatic moiré material is the magic-angle twisted bilayer/trilayer graphene (MATBG/TTG) [12], where correlated (Chern) insulators [13–21], unconventional superconductivity [13, 14, 22–35] with pseudogaps [36–38], and strange metal transport [39–41] are discovered. It is then realized that the topological flat bands [42–46] can be disentangled into itinerant Dirac bands (c) hybridizing with moiré local orbitals (f) [47–51]. Coulomb repulsion generates a large Hubbard $U \sim 60\text{meV}$ on each f orbital, which promotes the formation of local moments. Fermi liquid (FL) phases of heavy fermion or mixed-valence types can form via

the Kondo screening by the c electrons. Various phenomena get explained within this framework [52–63], including the Pomeranchuk effect [64–66], cascade transitions in scanning tunneling microscope (STM) spectrum [67, 68] and compressibility [32, 66, 69]. The coexistence of correlated f and light c is directly supported by thermoelectric transport [70] and the quantum twisting microscopy [71]. The Kondo resonance is also recently observed in STM [38].

The superconducting gap coexists with a larger pseudogap [37, 38], which appears at an energy scale of $1 - 4\text{meV}$, comparable to the phonon-mediated electron-electron interaction J [72–79]. In the Hilbert space of a local f -orbital, J induces anti-Hund’s splitting favoring spin-singlet configurations [80–84], in stark contrast to the atomic f shells, where the conventional Hund’s rule governs. Based on the assumption that a local FL emerges at an energy below $\mathcal{O}(J)$, a previous work demonstrates that quasiparticles experience an attractive renormalized interaction [1]. In addition, recent dynamical mean-field theory (DMFT) works also show that J leads to pseudogaps of size $\mathcal{O}(J)$ and different quantum phases [2]. These studies strongly indicate that the anti-Hund’s coupling can account for both pairing and pseudogap.

In this context, we consider a spin-valley Anderson impurity model (SVAIM) with a general valley-anisotropic (anti-)Hund’s interaction, which can describe a correlated orbital in the hetero-strained MATBG/TTG [85, 86]. We study its full phase diagram analytically, with support by numerical renormalization group (NRG) calculations, and analyze the occurrence of pairing and pseudogap.

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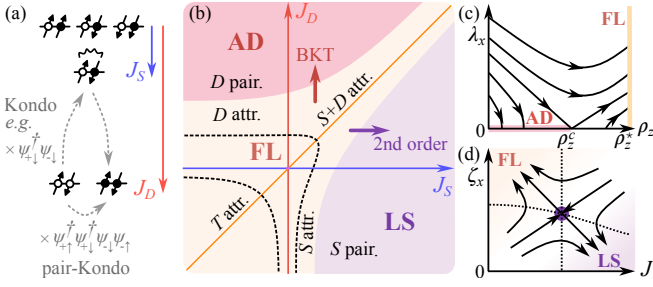


FIG. 1. (a) Energy diagram of the two-electron impurity states in SVAIM. White and black circles indicate valley $l = \pm$, respectively, and arrows indicate spin $s = \uparrow\downarrow$. J_S (J_D) is the energy decrease of the singlet S (the valley doublet D) compared to the spin triplet T ; see Eq. (1). (b) Schematic phase diagram of SVAIM. The FL phase is separated from the anisotropic doublet (AD) phase by a BKT transition, and separated from the local singlet (LS) phase by a second-order transition. Dashed lines mark the crossover boundaries of the sub-regions in the FL phase, where renormalized interactions turn attractive (“attr.”) in certain channels (S , D , or T). AD and LS also exhibit enhanced pairing (“pair.”) susceptibilities in the corresponding channels, despite no quasiparticle exists. (c, d) Schematic renormalization group flows for the BKT and second-order transitions, respectively. For NRG results corresponding to panels (b)–(d), see End Matter and Sec. I in Supplementary Material (SM) [87].

Model—Hetero-strain in MATBG/TTG lifts the otherwise degenerate orbital angular momenta of f [47] into bonding and anti-bonding levels [51], while leaving the valley ($l = \pm$) and spin ($s = \uparrow\downarrow$) symmetries intact. Upon electron (hole) doping, the bonding (anti-bonding) level remains frozen [61, 62], thus it suffices to model the active level, with electron operator f_{ls} . We introduce Pauli matrices σ^μ and ζ^ν ($\mu, \nu = 0, x, y, z$) for valley and spin, respectively. Besides charge- $U(1)$ symmetry generated by $\sigma^0\zeta^0$, there are spin- $SU(2)$ symmetry generated by $\zeta^{x,y,z}$, valley- $U(1)$ symmetry generated by σ^z , and a C_{2z} symmetry that interchanges the two valleys represented by σ^x .

The SVAIM is described by $H = H_0 + H_{\text{imp}} + H_c$. The bath Hamiltonian $H_0 = \int dx \sum_{ls} \psi_{ls}^\dagger(x) (i\partial_x) \psi_{ls}(x)$ is chosen as a chiral fermion for the convenience of analytical treatment, $H_c = \sqrt{2\Delta_0} \sum_{ls} f_{ls}^\dagger \psi_{ls}(0)$ is the hybridization between the impurity and bath states, and $H_{\text{imp}} = \frac{U}{2}(N - 2)^2 + H_{\text{AH}}$ is the impurity Hamiltonian. U is the Hubbard repulsion, N counts the impurity electron number, and H_{AH} is a general symmetry-allowed anti-Hund’s interaction. By symmetry, the two-electron subspace can split into a spin triplet (T), a valley doublet (D) carrying total valley charge $L^z = \pm 2$, and a singlet (S) [Fig. 1(a)]. Therefore, we parametrize

$$H_{\text{AH}} = -\frac{J_S}{2} \sum_{l'l''} f_{l'l}^\dagger f_{l'l}^\dagger f_{l''\downarrow} f_{l''\uparrow} - J_D \sum_l f_{l\uparrow}^\dagger f_{l\downarrow}^\dagger f_{l\downarrow} f_{l\uparrow} \quad (1)$$

which lowers the energy of S, D relative to T by $J_{S,D}$, respectively. $J_{S,D} > 0$ thus corresponds to an anti-Hund’s rule. Since $S \oplus D$ forms the “valley triplet” of a valley- $SU(2)$ group generated by $\sigma^{x,y,z}$, $J_S \neq J_D$ describes valley-anisotropy. As $J_{S,D}$ originate from phonon-mediated interactions, they are much weaker than the Coulomb repulsion U .

At energy $\omega \ll \mathcal{O}(U)$, charge fluctuations on f get frozen, turning into virtual processes that induce a Kondo coupling, $|\Xi\rangle\langle\Xi'| : \psi^\dagger \sigma^\mu \zeta^\nu \psi :$ (Sec. B 2 in SM [87]). $|\Xi\rangle$ runs over two-electron states, and $:\dots:$ normal-orders bilinear operators of bath electrons. The Kondo coupling strengths can be obtained via a Schrieffer-Wolff transformation. They are anti-ferromagnetic (> 0), and of order $\mathcal{O}(\frac{\Delta_0}{U})$.

Several limits are already well studied. $J_S = J_D = 0$ enjoys a full $SU(4)$ symmetry, and one channel of $SU(4)$ bath is known to exactly screen the $SU(4)$ impurity moment [53, 88, 89]. Increasing $J_S = J_D$ in either sign breaks $SU(4)$ into commuting spin- $SU(2)$ and valley- $SU(2)$ groups. As $J_S = J_D > 0$ grows, T gradually disappears from the low-energy space. Consequently, the bath spins $s = \uparrow\downarrow$ degrade to two degenerate channels that carry valley- $SU(2)$ moments to screen the valley triplet. The solution is also a FL [88, 90]. Physics at $J_S = J_D < 0$ is equivalent to $J_S = J_D > 0$, except with the roles of “spin” and “valley” exchanged. Since removing or recovering either triplet does not interrupt the exact screening, we conclude that the full diagonal line $J_S = J_D$ is FL.

As valley- $SU(2)$ is not guaranteed in real materials, $J_S \neq J_D$. Depending on which multiplet is the lowest, we divide the parameter space into three regimes. In the triplet regime ($J_{S,D} < 0$), splitting occurs in the high-energy subspace, not affecting FL at low energies. In the doublet ($0 < J_D, J_S < J_D$) or singlet ($0 < J_S, J_D < J_S$) regimes, however, splitting can eventually remove the Kondo resonance.

FL phase—For completeness, we discuss the FL phase first, which manifests a coherent Kondo peak in the impurity spectral function $A_f(\omega)$ at $\omega = 0$. The Kondo peak adiabatically evolves from the non-interacting resonant level ($U = J_{S,D} = 0$), leading to the formation of heavy quasiparticles at energies lower than the Kondo temperature T_K . T_K is the inverse of quasiparticle lifetime due to the hybridization with the bath. It decreases exponentially in increasing $\frac{U}{\Delta_0}$, and defines a universal energy scale in the low-energy end. By symmetry, the renormalized interactions between quasiparticles obey the same form as the bare ones, and we denote the renormalized parameters as $\tilde{U}$ and $\tilde{J}_{S,D}$. The quasiparticle susceptibilities of charge ($\sigma^0\zeta^0$), spin (ζ^z), and valley (σ^z) are then computed to the first order in $\tilde{U}$ and $\tilde{J}_{S,D}$ as (Sec. H 1 in [87]) [91–94]

$$\frac{\pi T_K}{4} \begin{pmatrix} \chi_c \\ \chi_s \\ \chi_v \end{pmatrix} = 1 - \frac{1}{\pi T_K} \begin{pmatrix} 3 & -1 & -\frac{1}{2} \\ -1 & 1 & \frac{1}{2} \\ -1 & -1 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \tilde{U} \\ \tilde{J}_D \\ \tilde{J}_S \end{pmatrix}. \quad (2)$$

No higher-order contributions arise from $\tilde{U}$ and $\tilde{J}_{S,D}$, as they are already fully renormalized. Crucially, because quasiparticles carry the same symmetry charges as the bare particles, the above relation gives the exact impurity susceptibilities, a result guaranteed by the Ward identity [95–97]. Knowledge of $\chi_{c,s,v}$ allows us to constrain $\tilde{U}$ and $\tilde{J}_{S,D}$.

By the strong U , charge fluctuation is always frozen at the Kondo energy scale, implying $\chi_c \ll T_K^{-1}$. In the $SU(4)$ symmetric limit, since $\tilde{J}_D = \tilde{J}_S = 0$, this constraint readily fixes

$\tilde{U} = \frac{\pi T_K}{3}$, meaning all channels are repulsive. Increasing $J_D = J_S = J$ until $J \gg T_K$, the impurity spin susceptibility also freezes, i.e., $\chi_s \ll T_K^{-1}$, leading to an attraction $\tilde{U} - \tilde{J} = -\frac{\pi T_K}{3}$ in the $S \oplus D$ channel. Between the two limits, χ_s interpolates smoothly, indicating a J_* where the $S \oplus D$ channel turns attractive, which we mark as a dashed line in Fig. 1(b). Reversely, the T channel turns attractive beyond $-J_*$ [94]. While interactions are irrelevant in a local FL, an attractive local vertex on the lattice problem can seed a pairing instability in the corresponding channel [1].

Doublet regime—The low-energy local Hilbert space consists of the doublet states $|L^z\rangle$ ($L^z = 2, \bar{2}$). We define Pauli matrices $\Lambda_z = |2\rangle\langle 2| - |\bar{2}\rangle\langle \bar{2}|$, and $\Lambda_+ = \Lambda_-^\dagger = |2\rangle\langle \bar{2}|$.

The only symmetry-allowed Kondo coupling in the low-energy space is $H_z = (2\pi\lambda_z)\Lambda_z : \psi^\dagger \sigma^z \zeta^0 \psi :|_{x=0}$, where the coupling constant $\lambda_z \sim \frac{\Delta_0}{U} > 0$ is anti-ferromagnetic. Crucially, $\Lambda_\pm$ cannot appear in the Kondo coupling, as they alter the impurity valley-charge by ± 4 , which cannot be compensated by a bilinear fermion operator of bath electrons. Nonetheless, two successive Kondo scatterings can first excite $|L^z\rangle$ to the S or T manifold, and then lower it to $|\bar{L}^z\rangle$ [Fig. 1(a)]. Such virtual multiplet fluctuations couple $\Lambda_\pm$ to a quartic bath operator, which scatters an electron pair at once. We thus dub it as the pair-Kondo (PK) coupling. Dictated by symmetries, it must take the form of

$$H_x = (2\pi)^2 \lambda_x x_c \cdot \Lambda_+ \cdot \psi_{-\uparrow}^\dagger \psi_{-\downarrow}^\dagger \psi_{+\downarrow} \psi_{+\uparrow} \Big|_{x=0} + h.c. \quad (3)$$

where λ_x is real-valued, and x_c is a microscopic length scale. A second-order perturbation theory estimates $\lambda_x \sim \mathcal{O}(\frac{\Delta_0^2}{U^2} \frac{1}{x_c J})$. Hereafter we always reserve J for the minimal multiplet excitation energy, which is $J = \min\{J_D, J_D - J_S\}$ in the doublet regime. The sign of λ_x does not affect the physics, as it can be changed by the gauge transformation $i\Lambda_z$. In sum, the effective Hamiltonian in the doublet regime is given by $H_{PK} = H_0 + H_z + H_x$.

We bosonize the chiral bath as $\psi_{ls}(x) \sim \frac{e^{-i\phi_{ls}(x)}}{\sqrt{2\pi x_c}}$ [98–106], where $\frac{1}{2\pi} \partial_x \phi_{ls}(x) =: \psi_{ls}^\dagger(x) \psi_{ls}(x)$ represents the electron density, hence $e^{-i\phi_{ls}(x)}$ serves as a Jordan-Wigner string that implements fermion anti-commutation within the same flavor. In H_{PK} , only one combination of boson fields, $\phi_v = \frac{1}{2} \sum_{ls} l \cdot \phi_{ls}$, couples to the impurity, which corresponds to the fluctuation of valley charges. The remaining three orthogonal channels decouple, including densities of electric charge (ϕ_c), spin (ϕ_s), and valley-contrasting spin (ϕ_{vs}). In subspaces that diagonalize $\Lambda_z = \pm$, H_z generates a phase shift of $l\Lambda_z \rho_z$ to each electron flavor ls , where $\rho_z = \frac{\arctan(\pi\lambda_z)}{\pi} \in (0, \frac{1}{2})$ [88, 102, 106], hence ϕ_v experiences a phase shift of $2\rho_z \Lambda_z$. A unitary transformation $\mathcal{U} = e^{i2\rho_z \Lambda_z \phi_v(0)}$ is then implemented to absorb this phase shift, such that $\bar{H}_{PK} = \mathcal{U} H_{PK} \mathcal{U}^\dagger = H_0 + \bar{H}_x$. H_0 still denotes the free chiral bath Hamiltonian, while the PK term

$$\bar{H}_x = \mathcal{U} H_x \mathcal{U}^\dagger = \frac{\lambda_x}{x_c} \cdot \Lambda_+ \cdot e^{-i(2-4\rho_z)\phi_v(0)} + h.c. \quad (4)$$

gets dressed by a phase factor of $4\rho_z \phi_v(0)$. The vertex operator $e^{i\gamma \phi_v(x)}$ has auto-correlation $\langle e^{-i\gamma \phi_v(0, \tau)} e^{i\gamma \phi_v(0, 0)} \rangle \sim$

$|\tau - \tau'|^{-\gamma^2}$, where $\phi_v(x, \tau) = e^{\tau H_0} \phi_v(x) e^{-\tau H_0}$. Therefore, $[e^{i\gamma \phi_v(x)}] = \frac{\gamma^2}{2}$ is termed as its scaling dimension. Here, $\gamma = 2 - 4\rho_z$. Under an RG action that coarse-grains $\tau \rightarrow \tau e^{d\ell}$, the scaling of λ_x is determined by the scaling dimension of the operator (Sec. D in SM [87]),

$$\frac{d\lambda_x}{d\ell} = \left(1 - \frac{\gamma^2}{2}\right) \lambda_x = (-1 + 8\rho_z - 8\rho_z^2) \lambda_x. \quad (5)$$

$\rho_z^c = \frac{1}{2} - \frac{1}{2\sqrt{2}} \approx 0.1464$ is thus a critical value, above which λ_x turns relevant.

ρ_z scales, too. $\bar{H}_x$ contributes a factor of $\langle T_\tau e^{-\int d\tau \bar{H}_x(\tau)} \rangle_0$ to the partition function, which can be expanded perturbatively in λ_x . The result can be mapped to a classical Coulomb gas [100, 107, 108] (Sec. D in SM [87]), where each flipping event $\Lambda_\pm$ is mapped to a particle on the τ axis with “electric charge” $\pm$, respectively, created with probability (fugacity) λ_x . γ^2 determines the inter-event correlations, and is mapped to the effective Coulomb strength. RG proceeds as two particles move close to form a dipole, which screens the Coulomb interaction among remaining particles, implying $\frac{d(\gamma^2)}{d\ell} \propto -\lambda_x^2 \gamma^2$. Further examination finds the proportionality as 4 (Sec. D in SM [87]), namely,

$$\frac{d\rho_z}{d\ell} = (1 - 2\rho_z) \lambda_x^2. \quad (6)$$

Since $\rho_z \in (0, \frac{1}{2})$, ρ_z always grows. Equations (5) and (6) are exact in ρ_z , but approximate to $\mathcal{O}(\lambda_x^3)$ order. The RG flow is drawn in Fig. 1(c), belonging to the Berezinskii–Kosterlitz–Thouless (BKT) type [109, 110].

There is a continuous fixed line with $\lambda_x = 0$ and arbitrary $\rho_z < \rho_z^c$, which we term as the AD phase. Beyond ρ_z^c , λ_x grows into a strong-coupling regime. We will soon show that an analytically solvable line [98, 99, 101, 103] exists at $\rho_z^* = \frac{1}{4}$, confirming the phase as FL.

BKT transition also occurs in the exemplary anisotropic Kondo problem (AK) [104, 107, 108]. Our AD line resembles the ferromagnetic line in AK, except that ρ_z^c in the latter case is zero. The difference originates from that the PK coupling is a quartic operator hence λ_x is irrelevant at the tree level, while the Kondo coupling in AK is marginal. Therefore, an infinitesimal anti-ferromagnetic ρ_z in AK suffices to drive the system into strong-coupling, while a threshold anti-ferromagnetic ρ_z^c in PK is required. It is the finite ρ_z^c that allows AD to appear in an Anderson model, where the effective ρ_z is always anti-ferromagnetic.

FL in doublet regime—At $\rho_z^* = \frac{1}{4}$ and arbitrary λ_x , the vertex operator appearing in Eq. (4) reads $e^{-i\phi_v(x)}$, hence can be re-fermionized as $\psi_v(x) \sim \frac{e^{-i\phi_v(x)}}{\sqrt{2\pi x_c}}$ [98–102]. To map Λ_- into another fermion f_v that anti-commutes with ψ_v , a Jordan-Wigner string that counts the total bath valley-charges is required (Sec. E in SM [87]). In the end, $\bar{H}_x = \sqrt{\frac{2\pi}{x_c}} \lambda_x f_v^\dagger \psi_v(0) + h.c.$, describing a resonant level f_v with zero on-site energy that hybridizes with ψ_v .

$\frac{\pi \lambda_x^2}{x_c}$ describes the resonance linewidth of f_v , to be identified as T_K . Below $T < T_K$, the impurity entropy freezes

to 0, and the static longitudinal susceptibility χ_v saturates to $\mathcal{O}(T_K^{-1})$, implying exact screening. We also solve the finite-size spectrum analytically (Sec. E in SM [87]), and find the impurity dynamic susceptibilities of Λ_z and $\Lambda_\pm$ (denoted as $\text{Im}\chi_z(\omega + i0^+)$ and $\text{Im}\chi_x(\omega + i0^+)$, respectively) to scale as $\sim \omega$ at $\omega \ll T_K$. These results also confirm FL behaviors.

Since bringing down S or T states into the low-energy Hilbert space does not interrupt the exact screening, FL in the doublet regime can cross over to FL in other regimes. Nevertheless, the renormalized interaction in the doublet regime behaves differently. A special limit is $J_S = 0$, where the global spin-SU(2) is enhanced into two independent SU(2) rotations in the two valleys $l = \pm$, generated by $\frac{\sigma^x \pm \sigma^z}{2} \zeta^{x,y,z}$. Such symmetry locks S and T as degenerate, namely $\tilde{J}_S = 0$. When $T_K \ll J_D$, charge and spin are almost frozen in the Fermi liquid, implying $\chi_c, \chi_s \ll T_K^{-1}$, solving which shows that D is the only attractive channel, with $\tilde{U} - \tilde{J}_D = -\pi T_K$ [111]. As splitting $J_S \neq 0$ in the high-energy end should not affect low-energy physics, the D channel will remain attractive as long as $T_K \ll J$.

Anisotropic doublet—At the fixed line ($\lambda_x = 0, \rho_z < \rho_z^c$), $\Lambda_z = \pm$ is conserved, implying its static susceptibility to exhibit the Curie's law, $\chi_v \sim T^{-1}$. On the other hand, $\Lambda_\pm$ is dressed by $\mathcal{U}\Lambda_\pm\mathcal{U}^\dagger = \Lambda_\pm e^{\pm i4\rho_z\phi_v(0)}$, where $\mathcal{U}$ is introduced above Eq. (4), implying its correlation function to scale as $\chi_x(\tau) \sim |\tau|^{-(4\rho_z)^2}$. Therefore, the dynamic susceptibility scales in a non-universal power law, $\text{Im}\chi_x(\omega + i0^+) \sim \text{sgn}(\omega)|\omega|^{16\rho_z^2-1}$, and the static susceptibility diverges as $\chi_x \sim T^{16\rho_z^2-1}$. The finite-size spectrum is given by chiral fermions with a phase shift $l\Lambda_z\rho_z$ (Sec. C in SM [87]).

The impurity spectral function $A_f(\omega)$ is proportional to the scattering $\mathcal{T}$ -matrix of bath electrons [112–114], and the latter remains well-defined in the downfolded model H_{PK} . According to the equation of motion $[H_z + H_x, \psi_{+\uparrow}(0)]$, $\psi_{+\uparrow}(0)$ scatters into two pieces: $\tilde{f}_{+\uparrow}^{(1)} = \lambda_z \Lambda_z \psi_{+\uparrow}|_{x=0}$ and $\tilde{f}_{+\uparrow}^{(2)} = (2\pi\lambda_x x_c) \Lambda_- \psi_{+\downarrow}^\dagger \psi_{-\downarrow} \psi_{-\uparrow}|_{x=0}$, where $\lambda_{z,x}$ should be understood as the un-renormalized parameters of H_{PK} . The scattering $\mathcal{T}$ -matrix is then given by the Green's function of $\tilde{f}^{(1)} + \tilde{f}^{(2)}$, whose long-time behavior is governed by the AD fixed point Hamiltonian. As Λ_z is conserved there, $\tilde{f}_{+\uparrow}^{(1,2)}$ do not mix. The time-evolution of $\tilde{f}_{+\uparrow}^{(1)}$ is solely governed by $\psi_{+\uparrow}$, which produces a spectrum proportional to the bath density of states, $A_f^{(1)}(\omega) \sim \text{const.}$ On the other hand, $\tilde{f}_{+\uparrow}^{(2)}$ is dressed by a non-universal phase factor as $\mathcal{U}\tilde{f}_{+\uparrow}^{(2)}\mathcal{U}^\dagger \sim \Lambda_- e^{-\frac{i}{2}(\phi_c + \phi_s + \phi_{vs})} e^{i(\frac{3}{2} - 4\rho_z)\phi_v}|_{x=0}$. Its Green's function hence scales as $|\tau|^{-\alpha_2}$, with $\alpha_2 = \frac{3}{4} + (\frac{3}{2} - 4\rho_z)^2$, implying a spectral function $A_f^{(2)}(\omega) \sim |\omega|^{\alpha_2-1}$. $0 < \rho_z < \rho_z^c$ maps to $2 > \alpha_2 - 1 > 2 - \sqrt{2} \approx 0.5858$ monotonically, hence near the BKT transition ρ_z^c , $A_f^{(2)}(\omega)$ behaves as a non-analytic kink depicted in Fig. 2(a), which contrasts significantly to the Kondo peak in FL.

Local pairing susceptibility in the D channel is found enhanced in the AD phase by Ref. [2]. We find this is due to the residual PK coupling λ_x [Eq. (4)] at intermediate energy

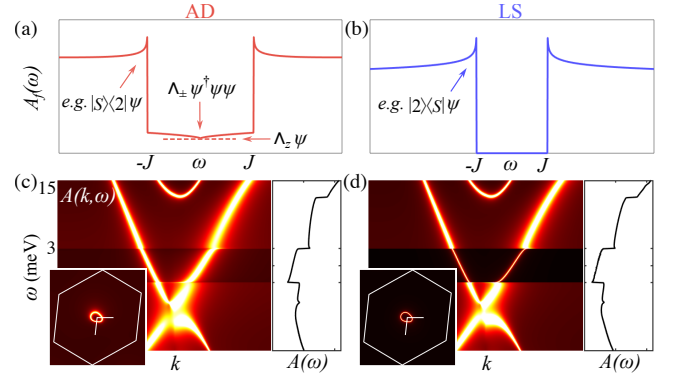


FIG. 2. (a, b) $A_f(\omega)$ obtained from bosonization. Pseudogap shoulders ($A_f^{(3)}$) correspond to multiplet excitations induced by scattering a bath electron ($\omega \leq -J$) or hole ($\omega \geq J$), hence are symmetrically pinned around the Fermi energy. For AD, residual longitudinal coupling contributes a constant background ($A_f^{(1)}$, dashed line), while the irrelevant PK coupling contributes a non-analytic kink ($A_f^{(2)}$) above it. (c, d) Lattice spectral function $A(k, \omega)$ in one valley, obtained using the *ansätze* of $\Sigma_f(\omega)$ derived from single impurity. Insets are contours at $\omega = 0$, with hexagons denoting the strained moiré Brillouin zone, and white lines indicating the k -path of main figures. AD does not have a well-defined Fermi surface, while LS is a Fermi liquid of c electrons. The total density of states $A(\omega) = \int \frac{d^2k}{(2\pi)^2} A(k, \omega)$ is also plotted.

scales, which couples the impurity to a bath electron pair in the D channel, and allows such pair excitations to lower energy by forming a singlet with the impurity (Sec. H2 in SM [87]). Meanwhile, an individual bath electron cannot benefit from such effect. Therefore, as the PK model inherits the symmetry charges of the Anderson model, while the residual charge fluctuation on f has been absorbed into the bath, such a pairing enhancement in the bath also reflects a pairing enhancement on f . It will thus be interesting for future work to investigate whether such “attraction” can lead to superconductivity on the lattice.

Pseudogap—Following the same reasoning, we investigate $A_f(\omega)$ at $\omega \sim \mathcal{O}(J)$, where the effective theory is the Kondo Hamiltonian. For simplicity, let us assume $0 < J_S < J_D$, and first include S into the low-energy space, so that the Kondo Hamiltonian reads $H_K = H_0 + H_J + H_z + H_{x0}$. $H_J = J|S\rangle\langle S|$ denotes the multiplet excitation with $J = J_D - J_S$, and the Kondo coupling between S and D reads $H_{x0} = (2\pi\zeta_x)\Theta_+ : \psi^\dagger \sigma^- \zeta^0 \psi : + h.c.$, where $\sigma^\pm = \frac{\sigma^x \pm i\sigma^y}{2}$, and $\Theta_+ = \Theta_-^\dagger = |S\rangle\langle 2| + |2\rangle\langle S|$. Therefore, $\psi_{+\uparrow}(0)$ also scatters into $\tilde{f}_{+\uparrow}^{(3)} = (2\pi\zeta_x)\Theta_- \psi_{-\uparrow}$, whose motion will contribute an $A_f^{(3)}(\omega)$. Note that the phase shift dresses $\tilde{f}_{+\uparrow}^{(3)}$ into $\mathcal{U}\tilde{f}_{+\uparrow}^{(3)}\mathcal{U}^\dagger \sim \Theta_- \cdot e^{-\frac{i}{2}(\phi_c + \phi_s - \phi_{vs})} e^{i(\frac{1}{2} - 2\rho_z)\phi_v}|_{x=0}$. Since Θ_- excites D to S , the minimal energy cost is J , leading to a factor $\theta(|\omega| - J)$ in $A_f^{(3)}(\omega)$. Meanwhile, the correlation function of the bath part scales as $|\tau|^{-\alpha_3}$, with $\alpha_3 = \frac{3}{4} + (\frac{1}{2} - 2\rho_z)^2 < 1$. Consequently, we find $A_f^{(3)}(\omega) \sim \theta(|\omega| - J)|\omega|^{-\alpha_3-1}$, forming the pseudogap shoulder [Fig. 2(a)]. Since terms irrelevant

at the AD fixed point can be important at such a high energy scale, quantitative behaviors around the shoulders can be altered. For example, the sharp step function $\theta(|\omega| - J)$ could be broadened. Further including T will bring in another set of shoulders at $\omega = \pm J_D$.

Singlet regime—Unlike the doublet regime, if the low-energy space is restricted to S , the impurity will have no internal degrees of freedom to interact with the bath, hence decouple. We term this phase as LS. To study the transition from FL to LS, we put back D (assuming $J_D > 0$, $J = J_S - J_D > 0$) and consider H_K presented in the last paragraph, except with replacing H_J with $J\Lambda_z^2$. Since J has the dimension of energy ($[J] = 1$), it grows under RG without ζ_x . For any $\rho_z > 0$, the Kondo coupling ζ_x has a relevant scaling dimension as well, as discussed for the AK model above. However, since a large ζ_x tends to overcome the excitation cost of J , while a large J suppresses the scattering amplitude of ζ_x , they generate quantum corrections that reduce each other. By this competition, FL and LS are separated by an unstable critical point, with a flow diagram depicted in Fig. 1(d) (Sec. F in SM [87]). This phase transition is consistent with previous NRG studies in similar models [111, 115, 116], where the critical point is found to be described by a non-Fermi liquid with impurity entropy $\ln\sqrt{2}$ [115]. When $J_D < 0$, the low-energy Hilbert space consists of $S \oplus T$, and the phase transition should be equivalent to that in the two-impurity Kondo problem [117–124], which was also found to be second-order.

As the S state carries no symmetry charge, $\chi_{c,s,v}$ are all frozen ($\ll T_K^{-1}$) in FL if $T_K \ll J$. Solving Eq. (2) finds the S channel is the only attractive one in the renormalized interaction, with $\tilde{U} - \tilde{J}_S = -3\pi T_K$ [116]. In the LS phase, Ref. [2] also find the local pairing susceptibility in S channel gets enhanced. Deep in LS phase, this can be shown by a perturbative calculation that integrates out the multiplet fluctuations, where the attractive strength is of $\mathcal{O}(\frac{\Delta_0^2}{U^2} \frac{1}{x_c J})$ (Sec. H2 in SM [87]).

The fixed-point Hamiltonian of LS only contains H_0 , hence $A_f(\omega) \rightarrow 0$ as $\omega \rightarrow 0$, in stark contrast to the in-gap excitations of AD. (Particle-hole asymmetry will lead to a small finite $A_f(0)$, see Sec. G1 in SM [87], but does not affect the pole in Σ_f ; see below.) The pseudogap shoulders, however, form by the same mechanism as in AD, as multiplet excitations to the D or T states induced by scattering a bath electron or hole [Fig. 2(b)].

Discussion—The single-impurity phase diagram [Fig. 1(b)] provides useful insights into the correlated phases in moiré lattices described by models of the heavy fermion type [47–51, 125]. In separate papers [2, 126], we show that quantum phase transitions into the AD and LS phases exhibiting pseudogap can indeed appear in the DMFT solution of MATBG [47] at filling fractions ν around ± 2 , if the corresponding anti-Hund’s rule is present. For a sketchy understanding to such lattice solutions, we construct analytic *ansatz* for the correlation self-energy $\Sigma_f(\omega)$ that reproduces the single-impurity

$A_f(\omega)$ (see End Matter), and insert it into the lattice Green’s function. Local FL leads to a heavy Fermi liquid on the lattice [52–59], with a Fermi volume $\frac{\nu}{4} = \frac{\nu_c + \nu_f}{4}$, where both f and c electrons contribute. If $T_K \ll J$, pseudogap shoulders at $\omega \sim \mathcal{O}(J)$ [similar to Fig. 2(a,b)] due to multiplet excitations can also be found, besides the Kondo resonance peak at $\omega = 0$. Increasing J_S locks each impurity into a LS, and we find $\Sigma_f \sim \frac{1}{\omega}$ at $\omega \ll J$, which gaps out the heavy f quasiparticles. Correspondingly, the Fermi volume jumps to $\frac{\nu - 2\text{sgn}(\nu)}{4}$ [Fig. 2(d)] [127], where $\nu_f \approx \pm 2$ disappears. If $\nu = 2$, the LS phase corresponds to a symmetric Mott phase [2, 83, 126, 128]. Contrarily, on increasing J_D into the AD phase, an unscreened doublet per unit cell remains. At finite temperature where no spontaneous symmetry breaking occurs, the in-gap excitations of A_f pervade the Brillouin zone, and also incur a finite lifetime to the c bands [Fig. 2(c)].

On lowering temperature, superconductivity may develop from different normal states, due to the local pairing potential in channels summarized in Fig. 1(b), forming a lower superconducting tunneling gap. Together with the higher pseudogap [Fig. 2], they provide potential explanation to the two-gap structure found by Refs. [37, 38]. Simultaneously, in the anti-Hund’s regime ($J_{S,D} > 0$), the valley moments spanned by $S \oplus D$ also couple to one another via Ruderman–Kittel–Kasuya–Yosida (RKKY) interactions. When the RKKY interaction is strong, the valley moments can align, leading to spontaneous symmetry breaking into either valley-polarized or inter-valley-coherent (IVC) [20, 21] states, which can co-exist with superconductivity. To clarify the interplay between superconductivity and IVC orders will be a crucial next step toward a complete theory of MATBG/TTG.

Note added—After posting this work, we became aware of a related study [129] that shares a similar perspective on the origin of pairing and pseudogap in MATBG.

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End Matter

Ansätze for correlation self-energy in AD and LS phases—Hubbard bands due to f charge fluctuation can be approximated as poles as $A_f^{(\text{at})}(\omega) = \frac{1}{2}\delta(\omega - \Delta E_L) + \frac{1}{2}\delta(\omega - \Delta E_U)$ [130], where $\Delta E_L < 0 < \Delta E_U$ and $\Delta E_U - \Delta E_L \approx U$. We write the total $A_f(\omega)$ as a mixing of $A_f^{(\text{at})}(\omega)$ and the $A_f^{(1,2,3)}(\omega)$ components defined above. To guarantee proper normalization, we also add smooth high-energy cutoffs to $A_f^{(1,2,3)}(\omega)$. We treat the positions of Hubbard peaks $\Delta E_{L,U}$, as well as the mixing amplitudes of each component, as tuning parameters in our ansätze. We then obtain $G_f(\omega)$ via the Kramer-König relation, and the self-energy via $\Sigma_f(\omega) = \omega - G_f^{-1}(\omega)$. Within the DMFT approximation that neglects spatial correlations, the lattice spectral function is given by $A(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{1}{\omega - H(k) - \Sigma_f(\omega + i0^+)}$, where $H(k)$ is the topological heavy fermion (THF) Hamiltonian of MATBG with hetero-strain (Sec. G3 in SM [87]).

Our *ansätze* are natural generalizations of the Hubbard-I approximation (HIA) [130–132], where $A_f = A_f^{(\text{at})}$. As $A_f^{(1,2,3)}(\omega)$ are included, we are able to capture the pseudogap and in-gap excitations, in addition to the Hubbard bands in MATBG [132] that are also captured by other approaches [133, 134].

Several remarks are in order. In the THF model, the hybridization strength Δ_0 of the quantum impurity problem is not determined by the $f^\dagger c$ hopping strength γ , but by the hybridization function $\sim \gamma^2 N(\omega)$, where $N(\omega)$ is the density of states. The AD and LS phases can exist in the $\gamma^2 N(\omega) \ll U$ limit even if $U \lesssim \gamma$. Moreover, in the LS phase, the poles corresponding to c bands will hybridize with the f Hubbard bands. If the f Hubbard bands are at high energy, the influence of hybridization will be weak [Fig. 2(d) or Fig. 3(a)]. If the f Hubbard bands are low, however, hybridization can strongly suppress the Fermi velocity, and the quasiparticle poles near the Fermi energy will also acquire significant f weights [Fig. 3(b)]. However, as it is an approximation to treat Hubbard bands as poles as in HIA, while physically they are broadened, it should be studied in the future whether the excitations with strong hybridization to Hubbard bands can still remain well-defined quasiparticles.

NRG calculations—We perform NRG calculations [113, 135] using the MuNRG toolbox [136, 137] based on the QSpace tensor library [138, 139]. We exploit the charge- $U(1)$, valley- $U(1)$, and spin- $SU(2)$ symmetries. Unless otherwise specified, we keep ~ 3000 multiplets (~ 8000 states). The Wilson chain is constructed with a discretization parameter $\Lambda = 3$. The z -averaging technique [140–142] with $n_z = 2$ is employed for calculating the correlation functions. We fix the Hubbard repulsion $U = 3$, and use a box-shaped hybridization function $\Delta(\omega) = \Delta_0 \theta(D - |\omega|)$ with $\Delta_0 = 0.2$ and $D = 10$.

The NRG phase diagram is plotted in Fig. 4(a). The three phases are distinguished by different fixed-point NRG spectra. FL and LS are both Fermi-liquid-like, but with opposite even-odd oscillations, corresponding to the $\frac{\pi}{2}$ and 0 phase shifts of bath electrons, respectively. The AD phase simply

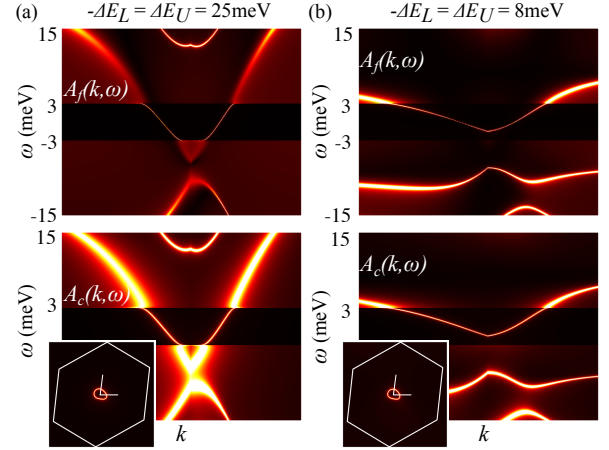


FIG. 3. Lattice spectral function in the LS phase, plotted component-wise, $A(k, \omega) = A_f(k, \omega) + A_c(k, \omega)$. (a) Same as Fig. 2(d), but with a different k -path (inset). Both Hubbard peaks of f lie at high energies ± 25 meV, thus the Fermi surface majorly comprises of c . (b) Lowering the Hubbard peaks to ± 8 meV. Although the Fermi volume is still given by $\frac{\nu-2}{4}$ (inset), hybridization between c bands and the f Hubbard bands has strongly suppressed the Fermi velocity.

exhibits non-universal phase shift ρ_z . $A_f(\omega)$ differs as well. FL, LS, and AD exhibits a sharp resonance peak, a full gap with $A_f(0) = 0$, and a gap with $A_f(0) \neq 0$, respectively, consistent with the analytical results. See Sec. I1 in SM [87] for typical RG flow and impurity spectral function in these phases.

In NRG, we define T_K in the FL phase by the renormalized hybridization $T_K = \tilde{\Delta}_0 = z\Delta_0$, where $z = [1 - \partial_\omega \Sigma_f(\omega)|_{\omega=0}]^{-1}$ is the quasiparticle weight. z is calculated by fitting the renormalized chain parameters [93] as detailed in Sec. I2 in SM [87]. We find that, generically speaking, T_K is higher if the impurity ground state degeneracy is higher. For example, a “ridge” of T_K extends along the line $J_D = J_S > 0$, where S and D are degenerate; along the line $J_S = 0 > J_D$, where S and T are degenerate; and along the line $J_D = 0 > J_S$, where D and T are degenerate.

In the FL phase, we extract the renormalized parameters $\tilde{U}, \tilde{J}_D, \tilde{J}_S$ from the NRG spectra [93], as explained in Sec. I2 in SM [87]. The effective interaction strengths in S, D, T channels, $\tilde{E}_S = \tilde{U} - \tilde{J}_S, \tilde{E}_D = \tilde{U} - \tilde{J}_D, \tilde{E}_T = \tilde{U}$ are shown in Fig. 4(b)–(d), where the attractive regions agree with Fig. 1(b). Three linecuts, $J_S = 0, J_D = 0.05$, and $J_S = J_D$ are plotted in Fig. 4(e)–(g), in order to better illustrate that the interaction strengths indeed asymptote to the Ward identity results as $T_K \rightarrow 0$ (Table I).

Renormalized parameters can also be defined in the LS phase, where the bath still forms a Fermi liquid. As the impurity decouples in the low-energy regime, we regard the first bath site in NRG as a new “impurity”, following Ref. [111] (Sec. I2 in SM [87]). As shown in Fig. 4(f), renormalized parameters obtained in FL and LS phases both asymptote to

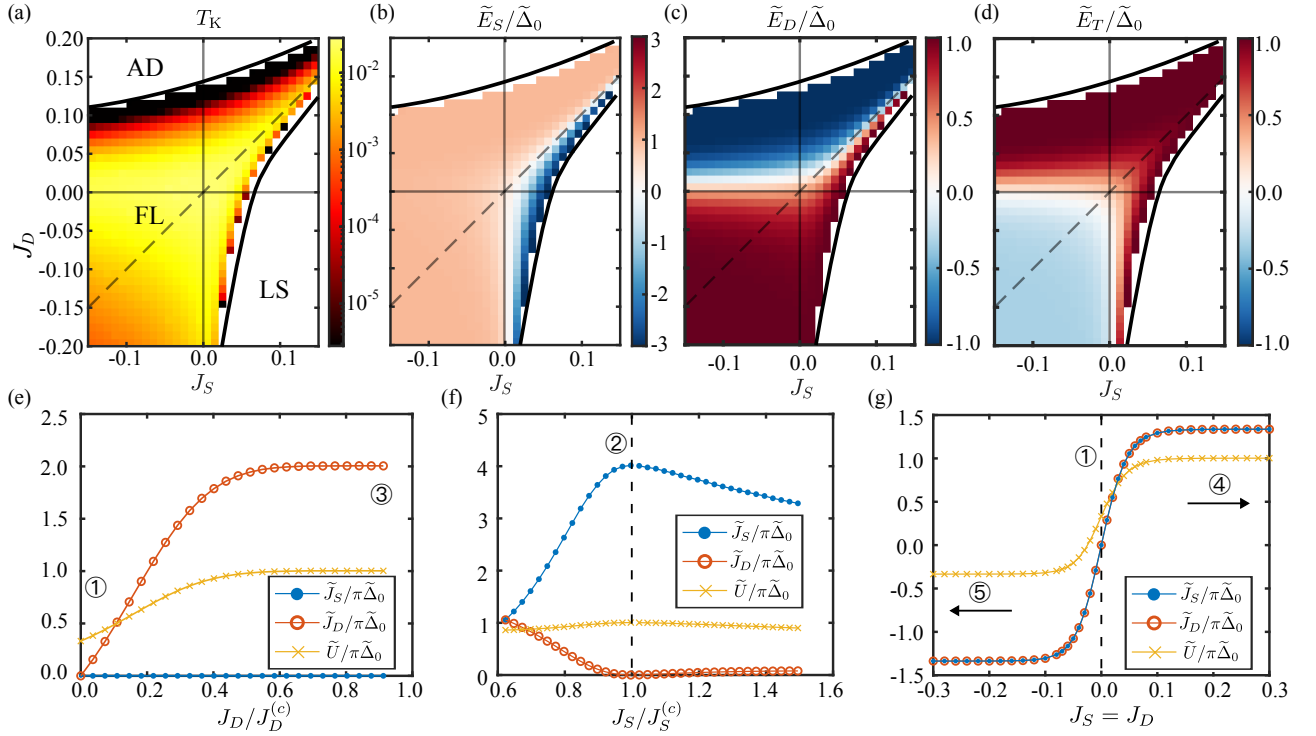


FIG. 4. NRG results of the phase diagram, T_K , and effective parameters of the SVAIM. (a) Phase diagram on (J_S, J_D) plane. The black solid lines sketch the phase boundary, and the color in the FL phase indicates T_K . The grey dashed line marks $J_S = J_D$. (b)-(d) The effective interactions in S, D, T channels $\tilde{E}_{S,D,T}$ compared to $\tilde{\Delta}_0$ as a function of J_S, J_D in the FL phase. (e)-(g) $\tilde{J}_S/\pi\tilde{\Delta}_0, \tilde{J}_D/\pi\tilde{\Delta}_0, \tilde{U}/\pi\tilde{\Delta}_0$ as functions of: (e) $J_D/J_D^{(c)}$ when $J_S = 0$, (f) $J_S/J_S^{(c)}$ when $J_D = 0.05$, (g) J_S when $J_S = J_D$. The dashed lines in (f),(g) mark the FL-LS critical point and $J_S = J_D = 0$, respectively. The numeric labels indicate the regions where the relations in Table I hold, while the arrows in (g) show that these relations remain valid upon increasing $|J_S|$ along the line $J_S = J_D$.

Parameter region	Impurity GS	$\frac{1}{\pi T_K}(\tilde{E}_S, \tilde{E}_D, \tilde{E}_T)$
① $U \gg T_K; J_D = J_S = 0$	$S \oplus D \oplus T$	$(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$
② $J_S, J_S - J_D, U \gg T_K$	S	$(-3, 1, 1)$
③ $J_D, U \gg T_K; J_S = 0$	D	$(1, -1, 1)$
④ $J_S, U \gg T_K; J_S = J_D > 0$	$S \oplus D$	$(-\frac{1}{3}, -\frac{1}{3}, 1)$
⑤ $ J_S , U \gg T_K; J_S = J_D < 0$	T	$(1, 1, -\frac{1}{3})$

TABLE I. Renormalized FL parameters by Ward identities. The five parameter regions are marked in Fig. 4(e)-(g). Notice that besides the attractive channel favored by the lowest-lying impurity multiplet, other channels are equally repulsive.

the Ward identity result when approaching the second-order critical point. Deep in the LS phase, the perturbative analysis to the effective bath interaction applies.

The scaling of T_K near phase transitions indicates the nature of the phase transitions. We select two linecuts, $J_S = 0$ [Fig. 5(a)] and $J_D = 0.05$ [Fig. 5(b)], to illustrate the BKT and the second-order transitions, respectively. For BKT, T_K can be

fitted by $T_K \propto e^{-c \sqrt{\frac{\Delta_0}{J_D^{(c)} - J_D}}}$ with some constant c , consistent with our analytical RG calculation and previous numerical re-

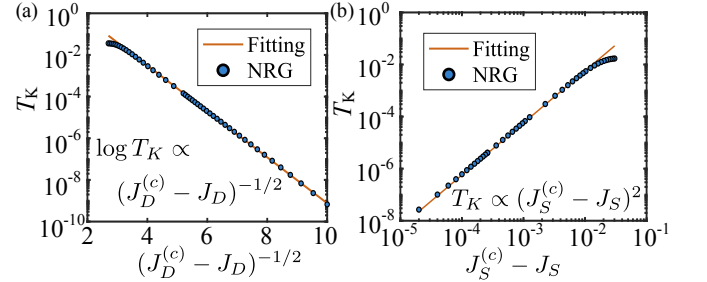


FIG. 5. T_K near the phase transitions. (a) BKT type, obtained along $J_S = 0$, with critical $J_D^{(c)} \approx 0.137$. (b) Second-order, obtained along $J_D = 0.05$, with critical $J_S^{(c)} \approx 0.08026$.

sults [109]. In Sec. 12 of SM [87], we further show that from the finite-size NRG spectrum flow, we can numerically extract the flow diagram of λ_x, λ_z , as plotted in Fig. 12(d), validating Fig. 1(c). On the other hand, T_K near the second-order transition can be fitted by $T_K \propto (J_S^{(c)} - J_S)^2$, consistent with our analytical RG calculation and previous numerical results [111, 115, 116].

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A. Bosonization-refermionization dictionary

To apply the bosonization technique to the impurity problem, we linearize the dispersion of bath electrons near the Fermi surface, extend the band width to infinity, and only keep the s -wave bath states that interact with the impurity. This effectively reduces the bath to 1-dimensional chiral fermions.

For the bosonization identities, we follow the constructive approach in Refs. [101–103]. We will treat the Klein factors that carry the quantum numbers in an exact manner, which helps keep track of the physical states in the enlarged Hilbert space. We

also keep the $\mathcal{O}(L^{-1})$ terms to analyze the finite-size spectrum, where L denotes the bath system size. But we will ignore them when calculating physical quantities in the thermodynamic limit, such as the partition functions and correlation functions.

For all the models studied in this work, the Fermi velocities of all bath flavors will be dictated by symmetries to be degenerate, hence we set them as $v_F = 1$. We also set the Planck constant $\hbar = 1$, elementary charge $|e| = 1$, and the Boltzmann constant $k_B = 1$, so all physical quantities can be measured in terms of the energy dimension.

1. Operator identity

Let α label the flavor of bath electrons. The chiral fermions can be formally put on a circle of length L , hence the finite-size energy spacing between two adjacent single-electron levels is $\frac{2\pi}{L}$. The Hamiltonian reads,

$$H_0 = \sum_k \sum_\alpha k : d_\alpha^\dagger(k) d_\alpha(k) : \quad k \in \frac{2\pi}{L} \left(\mathbb{Z} - \frac{P_{bc}}{2} \right) \quad (A1)$$

with $\{d_\alpha^\dagger(k), d_\alpha(k')\} = \delta_{kk'} \delta_{\alpha\alpha'}$, $\{d_\alpha(k), d_\alpha(k')\} = 0$. Here, $P_{bc} = 0, 1$ indicates whether the chemical potential lies exactly within a single-electron level, or between two levels. The normal-ordering of chiral fermions $: \cdots :$ is defined with respect to the following background $|0\rangle_0$,

$$d_\alpha(k)|0\rangle_0 = 0 \quad (\text{if } k > 0) \quad d_\alpha^\dagger(k)|0\rangle_0 = 0 \quad (\text{if } k \leq 0). \quad (A2)$$

Note that $|0\rangle_0$ occupies all *non-positive* levels including zero. The Fourier transformation to real-space reads

$$\psi_\alpha(x) = \sqrt{\frac{1}{L}} \sum_k d_\alpha(k) e^{-ikx}, \quad d_\alpha(k) = \sqrt{\frac{1}{L}} \int_{-\frac{L}{2}}^{\frac{L}{2}} dx \psi_\alpha(x) e^{ikx} \quad (A3)$$

with $\{\psi_\alpha^\dagger(x), \psi_{\alpha'}(x')\} = \delta(x - x') \delta_{\alpha\alpha'}$, $\{\psi_\alpha(x), \psi_{\alpha'}(x')\} = 0$. Since $P_{bc} = 0, 1$ also determines whether the boundary condition at $x = \pm \frac{L}{2}$ is periodic or anti-periodic, we term it as the boundary condition parameter. In the real-space, the Hamiltonian reads

$$H_0 = \int dx \sum_\alpha : \psi_\alpha^\dagger(x) (i\partial_x) \psi_\alpha(x) : \quad (A4)$$

The U(1) charge that counts the total particle number in each flavor α is defined as

$$N_\alpha = \sum_k : d_\alpha^\dagger(k) d_\alpha(k) : = \int dx : \psi_\alpha^\dagger(x) \psi_\alpha(x) : \in \mathbb{Z} \quad (A5)$$

Note that the chiral fermions are all *left-movers*, and, to keep a consistent notation with Ref. [101], we have adopted the convention $\psi_\alpha(x) \sim d_\alpha(k) e^{-ikx}$ such that $d_\alpha(k)$ is an eigenmode of the energy k . (If the more common convention $\psi_\alpha(x) \sim d_\alpha(k) e^{ikx}$ were adopted, $d_\alpha(k)$ would have an eigenenergy of $-k$.)

Bosonization relies on the fact that, any $\vec{N}$ -particle Fock state in the physical Hilbert space, where $\vec{N}$ collects all quantum numbers $N_\alpha \in \mathbb{Z}$ into a vector, can be constructed from a unique $\vec{N}$ -particle ground state $|\vec{N}\rangle_0$ by acting upon it a series of particle-hole excitations that commute with $\vec{N}$. All operators within the physical Hilbert space can thus be constructed from two types of elements: 1) the Klein factors F_α that link between $\vec{N}$ -particle *ground* states $|\vec{N}\rangle_0$ with different $\vec{N}$, and encode the fermion anti-commutation between different α , and 2) the bosonic fields $\phi_\alpha(x)$ that generate density fluctuations (i.e. particle-hole excitations) that commute with all $N_{\alpha'}$. Also, $[F_\alpha, \phi_{\alpha'}(x)] = 0$. We refer the detailed derivation of the bosonization procedures to Ref. [101], and only summarize the definitions and key identities below.

The fermion operator is bosonized to,

$$\psi_\alpha(x) = \frac{F_\alpha}{\sqrt{2\pi x_c}} e^{-i\phi_\alpha(x)} e^{-i\left(N_\alpha - \frac{P_{bc}}{2}\right) \frac{2\pi x}{L}}. \quad (A6)$$

Here, $x_c \rightarrow 0^+$ is an ultraviolet cutoff. We remark that the fermion Hilbert space (as well as the boson Hilbert space introduced below) is not truncated, and $x_c \rightarrow 0^+$ is only introduced to realize the operator identity. Sometimes x_c^{-1} can be interpreted as an “effective bandwidth” of the chiral fermion. F_α are Klein factors that obey

$$[N_\alpha, F_{\alpha'}] = -F_{\alpha'} \delta_{\alpha\alpha'}, \quad F_\alpha F_\alpha^\dagger = F_\alpha^\dagger F_\alpha = 1, \quad \{F_\alpha, F_{\alpha'}^\dagger\} = 2 \cdot \delta_{\alpha\alpha'}, \quad \{F_\alpha, F_{\alpha'}\} = 2F_\alpha^2 \cdot \delta_{\alpha\alpha'}. \quad (A7)$$

After specifying a certain ordering of the fermion flavors $\alpha = 1, 2, \dots$, we can define the normalized $\vec{N}$ -particle ground states as

$$|\vec{N}\rangle_0 = (F_1^\dagger)^{N_1} (F_2^\dagger)^{N_2} \dots |0\rangle_0. \quad (\text{A8})$$

where we take the convention that $(F_\alpha^\dagger)^{N_\alpha} = (F_\alpha)^{-N_\alpha}$ if $N_\alpha < 0$. Correspondingly, the matrix elements of Klein factors under the basis set $|\vec{N}\rangle_0$ read

$$F_\alpha |\vec{N}\rangle_0 = (-1)^{\sum_{\alpha' < \alpha} N_{\alpha'}} |\vec{N} - \Delta \vec{N}_\alpha\rangle_0 \quad \Delta \vec{N}_\alpha = (0, \dots, \frac{1}{\alpha_{\text{th}}}, \dots, 0) \quad (\text{A9})$$

where $(-1)^{\sum_{\alpha' < \alpha} N_{\alpha'}}$ is the Jordan-Wigner string due to the anti-commutation between Klein factors. It suffices to specify the action of F_α on the $\vec{N}$ -particle ground states, because all the bosonic operators that generate particle-hole excitations commute with F_α .

The bosonic field $\phi_\alpha(x)$ is defined as

$$\phi_\alpha(x) = \sum_{q>0} -\sqrt{\frac{2\pi}{qL}} \left(e^{-iqx} b_\alpha(q) + e^{iqx} b_\alpha^\dagger(q) \right) e^{-\frac{\pi c q}{2}} = \varphi_\alpha(x) + \varphi_\alpha^\dagger(x) \quad (\text{A10})$$

$$b_\alpha^\dagger(q) = i\sqrt{\frac{2\pi}{qL}} \sum_k d_\alpha^\dagger(k+q) d_\alpha(k), \quad q \in \frac{2\pi}{L} \mathbb{Z}_+ = \left\{ \frac{2\pi}{L}, 2\frac{2\pi}{L}, 3\frac{2\pi}{L}, \dots \right\} \quad (\text{A11})$$

By this definition, $\phi_\alpha(x)$ is always periodic under $x \rightarrow x+L$. Boson fields obey $[b_\alpha(q), b_{\alpha'}^\dagger(q')] = \delta_{\alpha\alpha'} \delta_{qq'}$, $[b_\alpha(q), b_{\alpha'}(q')] = 0$, and $[N_{\alpha'}, b_\alpha(q)] = 0$. We have also separately defined $\varphi_\alpha(x)$ and $\varphi_\alpha^\dagger(x)$, which are the components of $\phi_\alpha(x)$ that only consist of boson annihilation and creation operators, respectively.

We first compute the commutator

$$[\varphi_\alpha(x), \varphi_{\alpha'}^\dagger(x')] = \delta_{\alpha\alpha'} \sum_{n=1}^{\infty} \frac{1}{n} e^{(-i\frac{2\pi}{L}(x-x') - \frac{2\pi}{L}x_c)n} = -\delta_{\alpha\alpha'} \ln \left(1 - e^{-\frac{2\pi i}{L}(x-x'-ix_c)} \right), \quad (\text{A12})$$

where $\sum_{n=1}^{\infty} \frac{1}{n} y^n = -\ln(1-y)$ is used for $|y| < 1$. Hence

$$[\phi_\alpha(x), \phi_{\alpha'}(x')] = -\delta_{\alpha\alpha'} \ln \frac{1 - e^{-\frac{2\pi i}{L}(x-x'-ix_c)}}{1 - e^{-\frac{2\pi i}{L}(x'-x-ix_c)}} = -2i \cdot \delta_{\alpha\alpha'} \cdot \arg \left(1 - e^{-\frac{2\pi i}{L}(x-x')} e^{-\frac{2\pi}{L}x_c} \right). \quad (\text{A13})$$

Here, the single-valued branch of the above $\ln \dots$ function is always taken such that the commutator equals 0 if $x = x' \bmod L$, so that the $\arg(\dots)$ function takes values in $(-\frac{\pi}{2}, \frac{\pi}{2})$. Taylor-expanding Eqs. (A12) and (A13) with regard to $\frac{x-x'}{L}$ yields, respectively,

$$[\varphi_\alpha(x), \varphi_{\alpha'}^\dagger(x')] = \delta_{\alpha\alpha'} \left[-\ln \left(\frac{2\pi i}{L} (x-x'-ix_c) \right) + \frac{\pi i}{L} (x-x'-ix_c) \right] + \mathcal{O}(L^{-2}). \quad (\text{A14})$$

$$[\phi_\alpha(x), \phi_{\alpha'}(x')] = \delta_{\alpha\alpha'} \left[\ln \left(\frac{x'-x-ix_c}{x-x'-ix_c} \right) + \frac{2\pi i}{L} (x-x') \right] + \mathcal{O}(L^{-2}). \quad (\text{A15})$$

Notice that while Eqs. (A12) and (A13) are periodic in $x \rightarrow x+L$ and $x' \rightarrow x'+L$, the taylor-expanded Eqs. (A14) and (A15) are not. Hereafter we will omit $\mathcal{O}(L^{-2})$ terms in the real-space commutators, unless otherwise specified.

We write the commutator of the ϕ fields in a more commonly used form,

$$[\phi_\alpha(x), \phi_{\alpha'}(x')] = \delta_{\alpha\alpha'} \cdot (-\pi i) \cdot \left(\text{sgn}_{x_c}(x-x') - \frac{2}{L}(x-x') \right), \quad \text{sgn}_{x_c}(x) = \frac{2}{\pi} \arctan \frac{x}{x_c} \quad (\text{A16})$$

$$[\phi_\alpha(x), \partial_{x'} \phi_{\alpha'}(x')] = \delta_{\alpha\alpha'} \cdot (2\pi i) \cdot \left(\delta_{x_c}(x-x') - \frac{1}{L} \right), \quad \delta_{x_c}(x) = \frac{x_c}{\pi} \frac{1}{x^2 + x_c^2}, \quad (\text{A17})$$

where the single-branch of $\frac{1}{2i} \ln \frac{i-z}{i+z} = \arctan(z)$ is taken in such a way that $\arctan(0) = 0$.

Anti-commutation between fermion operators (Eq. (A6)) with different flavors is guaranteed by the Klein factors. We now verify the anti-commutation between fermion operators within the same flavor. First,

$$\begin{aligned} \psi_\alpha(x) \psi_\alpha(x') &= \frac{1}{2\pi x_c} F_\alpha \cdot e^{-i(N_\alpha - P_{bc}/2) \frac{2\pi}{L} x} \cdot F_\alpha \cdot e^{-i(N_\alpha - P_{bc}/2) \frac{2\pi}{L} x'} \cdot e^{-i\phi_\alpha(x)} e^{-i\phi_\alpha(x')} \\ &= \frac{1}{2\pi x_c} F_\alpha^2 \cdot e^{-i(N_\alpha - P_{bc}/2) \frac{2\pi}{L} (x+x')} \cdot e^{i\frac{2\pi}{L} x} \cdot e^{-i\phi_\alpha(x)} e^{-i\phi_\alpha(x')} \end{aligned} \quad (\text{A18})$$

where we have made use of $F_\alpha^\dagger N_\alpha F_\alpha = N_\alpha - 1$. By the Baker-Hausdorff formula

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}, \quad (\text{provided } [A, [A, B]] = [B, [A, B]] = 0) \quad (\text{A19})$$

and Eq. (A16), we have

$$\psi_\alpha(x)\psi_\alpha(x') = \frac{1}{2\pi x_c} F_\alpha^2 \cdot e^{-i(N_\alpha - P_{bc}/2)\frac{2\pi}{L}(x+x')} \cdot e^{i\frac{\pi}{L}(x+x')} \cdot e^{-i(\phi_\alpha(x)+\phi_\alpha(x'))} \cdot e^{i\frac{\pi}{2}\text{sgn}_{x_c}(x-x')} . \quad (\text{A20})$$

Notice that the second term in the $[\phi_\alpha(x), \phi_\alpha(x')]$ commutator (Eq. (A16)) changes the phase factor $e^{i\frac{2\pi}{L}x}$ to $e^{i\frac{\pi}{L}(x+x')}$. Given $x_c \rightarrow 0^+$, the above result immediately leads to $\{\psi_\alpha(x), \psi_\alpha(x')\} = 0$. One can similarly verify $\{\psi_\alpha(x), \psi_\alpha^\dagger(x')\} = 0$ for $x \neq x'$.

We then consider the operator $\psi_\alpha^\dagger(x)\psi_\alpha(x')$ in the $x' \rightarrow x$ limit. To simplify the calculation, we first rewrite the fermion operator in a normal ordered (with respect to boson vacuum) form

$$\psi_\alpha(x) = \frac{F_\alpha}{\sqrt{L}} e^{-i(N_\alpha - P_{bc}/2)\frac{2\pi}{L}x} e^{-i\varphi_\alpha^\dagger(x)} e^{-i\varphi_\alpha(x)} = \frac{F_\alpha}{\sqrt{L}} e^{-i(N_\alpha - P_{bc}/2)\frac{2\pi}{L}x} : e^{-i\phi_\alpha(x)} : \quad (\text{A21})$$

where we have made use of $e^{-i\varphi_\alpha^\dagger(x)-i\varphi_\alpha(x)} = e^{-i\varphi_\alpha^\dagger(x)} e^{-i\varphi_\alpha(x)} e^{\frac{1}{2}[\varphi_\alpha^\dagger(x), \varphi_\alpha(x)]}$ and $[\varphi_\alpha^\dagger(x), \varphi_\alpha(x)] = \ln \frac{2\pi x_c}{L}$. Here $: \dots :$ represents normal ordering with respect to the boson vacuum. Then we have

$$\begin{aligned} \psi_\alpha^\dagger(x)\psi_\alpha(x') &= \frac{1}{L} e^{i(N_\alpha - P_{bc}/2)\frac{2\pi}{L}x} F_\alpha^\dagger F_\alpha e^{-i(N_\alpha - P_{bc}/2)\frac{2\pi}{L}x'} \cdot e^{i\varphi_\alpha^\dagger(x)} e^{i\varphi_\alpha(x)} e^{-i\varphi_\alpha^\dagger(x')} e^{-i\varphi_\alpha(x')} \\ &= \frac{1}{L} e^{i(N_\alpha - P_{bc}/2)\frac{2\pi}{L}(x-x')} \cdot e^{i\varphi_\alpha^\dagger(x)} \left[e^{-i\varphi_\alpha^\dagger(x')} e^{i\varphi_\alpha(x)} \cdot e^{[\varphi_\alpha(x), \varphi_\alpha^\dagger(x')]} \right] e^{-i\varphi_\alpha(x')} \\ &= \frac{1}{2\pi i} \cdot \frac{1}{x - x' - ix_c} e^{i(N_\alpha - P_{bc}/2 + 1/2)\frac{2\pi}{L}(x-x')} \cdot e^{i(\varphi_\alpha^\dagger(x) - \varphi_\alpha^\dagger(x'))} e^{i(\varphi_\alpha(x) - \varphi_\alpha(x'))} . \end{aligned} \quad (\text{A22})$$

Taking $x_c \rightarrow 0^+$ first and then Taylor-expanding $x - x'$, we obtain

$$\begin{aligned} \psi_\alpha^\dagger(x)\psi_\alpha(x') &= \frac{1}{2\pi i} \frac{1}{x - x' - ix_c} + \frac{N_\alpha + 1/2 - P_{bc}/2}{L} + \frac{1}{2\pi} \partial_x \phi_\alpha(x) + \frac{x - x'}{4\pi} (i : (\partial_x \phi_\alpha(x))^2 : + \partial_x^2 \phi_\alpha(x)) \\ &\quad + i(x - x') \frac{N_\alpha + 1/2 - P_{bc}/2}{L} \partial_x \phi_\alpha(x) + \mathcal{O}((x - x')^2) . \end{aligned} \quad (\text{A23})$$

Recall that $\mathcal{O}(L^{-2})$ terms are also omitted. The normal ordered density operator, where the constant term $\frac{1}{2\pi i} \frac{1}{x - x' - ix_c} + \frac{1/2 - P_{bc}/2}{L}$ is removed, is then given by

$$: \psi_\alpha^\dagger(x)\psi_\alpha(x) : = \frac{1}{2\pi} \partial_x \phi_\alpha(x) + \frac{N_\alpha}{L} , \quad (\text{A24})$$

which is consistent with Eq. (A10).

We substitute Eq. (A23) into the kinetic energy Hamiltonian Eq. (A4) and obtain

$$H_0 = \sum_\alpha \int \frac{dx}{4\pi} (: (\partial_x \phi_\alpha(x))^2 : + \mathcal{O}(L^{-2})) . \quad (\text{A25})$$

Integral over full derivative terms, *e.g.*, $\partial_x \phi_\alpha$ and $\partial_x^2 \phi_\alpha$, vanishes due to the periodic boundary condition of the boson field. The omitted $\mathcal{O}(L^{-2})$ term in the integrand will contribute to an $\mathcal{O}(L^{-1})$ term to the total energy, which is of interest. To obtain this term, we consider the vacuum $|\vec{N}\rangle_0$ defined in Eq. (A8). Since the operator $: (\partial_x \phi_\alpha)^2 :$ kills $|\vec{N}\rangle_0$, the $\mathcal{O}(L^{-1})$ term determines the energy of $|\vec{N}\rangle_0$, which can be simply counted as $\sum_\alpha \sum_{n=1}^{N_\alpha} \frac{2\pi}{L} (n - P_{bc}/2) = \frac{2\pi}{L} \frac{N_\alpha(N_\alpha + 1 - P_{bc})}{2}$. Therefore, we conclude that the kinetic energy Hamiltonian is

$$\begin{aligned} H_0 &= \sum_\alpha \int \frac{dx}{4\pi} : (\partial_x \phi_\alpha(x))^2 : + \sum_\alpha \frac{2\pi}{L} \frac{N_\alpha(N_\alpha + 1 - P_{bc})}{2} \\ &= \sum_\alpha \sum_{q>0} q : b_\alpha^\dagger(q) b_\alpha(q) : + \sum_\alpha \frac{2\pi}{L} \frac{N_\alpha(N_\alpha + 1 - P_{bc})}{2} . \end{aligned} \quad (\text{A26})$$

Note that the $\mathcal{O}(L^{-1})$ term relies on the definition of $|0\rangle_0$, which is chosen to occupy all non-positive levels including zero.

We remark again that Eqs. (A6), (A16), (A17), (A24) and (A26) contain $\mathcal{O}(L^{-1})$ terms. We will keep these $\mathcal{O}(L^{-1})$ terms when discussing the finite-size spectrum and neglect them otherwise.

2. Phase shift due to δ -potential

Following Refs. [88, 102, 106], we discuss and compute the phase shift $\pi\rho$ generated by a δ -function potential of strength $\lambda \cdot 2\pi$. For this purpose, it suffices to consider a single-flavor problem, and drop the flavor index α in this subsection.

Phase shift—The second-quantized Hamiltonian reads,

$$H_0 + H_1 = \int dx : \psi^\dagger(x)(i\partial_x)\psi(x) : + \lambda \cdot (2\pi) : \psi^\dagger(0)\psi(0) : \quad (\text{A27})$$

which in the first-quantized language corresponds to an eigenvalue problem

$$(i\partial_x + \lambda \cdot 2\pi \cdot \delta(0))\psi(x) = k \cdot \psi(x) \quad (\text{A28})$$

It can be solved by the following ansatz (with the normalization factor ignored),

$$\psi(x) \sim e^{-ikx}e^{-i\pi\rho} \quad (\text{if } x < 0) \quad \psi(x) \sim e^{-ikx}e^{i\pi\rho} \quad (\text{if } x > 0) \quad (\text{A29})$$

with the phase shift $\pi\rho$ to be determined. But the relation between ρ and λ depends on how one regularizes the delta potential at the high-energy end.

Following the discussions in Ref. [102], we regularize the delta potential as

$$H_1 = (\lambda \cdot 2\pi) \int dx \delta_{x_c}(x) \int dx' \delta_{x_c}(x') : \psi^\dagger(x)\psi(x') : \quad (\text{A30})$$

x_c restricts us to such processes where the momenta k' and k of both the incoming and outgoing electrons are individually within a cutoff $\mathcal{O}(x_c^{-1})$, which can be understood as a zero-range potential in a finite-width band. If one were to choose another regularization $H_1 = (\lambda \cdot 2\pi) \int dx \delta_{y_c}(x) : \psi^\dagger(x)\psi(x) :$, which only dictates the momentum difference $k - k'$ to be within $\mathcal{O}(y_c^{-1})$, and can be understood as a finite-range (y_c) potential in an infinite-width band ($y_c \gg x_c$), then the $\rho(\lambda)$ relation would be different. We will mainly focus on the first scheme.

Corresponding to the regularization scheme Eq. (A30), the first-quantized eigen-value problem is given by

$$i\partial_x\psi(x) + (\lambda \cdot 2\pi) \cdot \delta_{x_c}(x) \int dx' \delta_{x_c}(x') \psi(x') = k \cdot \psi(x) \quad (\text{A31})$$

For electrons far below the cutoff, $kx_c \rightarrow 0^+$, using the ansatz Eq. (A29), $\int dx' \delta_{x_c}(x') \psi(x') = \frac{\psi(0^-) + \psi(0^+)}{2}$ is an average of $\psi(0^-)$ and $\psi(0^+)$. Therefore, by further integrating Eq. (A31) over an infinitesimal region containing $x = 0$, we can solve the phase shift

$$i(\psi(0^+) - \psi(0^-)) + (\lambda \cdot 2\pi) \frac{\psi(0^+) + \psi(0^-)}{2} = 0 \quad \implies \quad \rho = \frac{\arctan(\lambda\pi)}{\pi} \in \left(-\frac{1}{2}, \frac{1}{2}\right). \quad (\text{A32})$$

In the second regularization scheme, we can similarly derive an eigen-equation, i.e., $i\partial_x\psi(x) + (\lambda \cdot 2\pi)\delta_{y_c}(x)\psi(x) = k \cdot \psi(x)$, and obtain the phase shift $\rho = \lambda$.

In terms of the finite-size spectrum, the phase shift also manifests as a global shift of all single-electron levels. Specifically, if one fixes $\psi(-\frac{L}{2}) = e^{-i\pi P_{bc}} \cdot \psi(\frac{L}{2})$, then the momentum k in Eq. (A29), which is also the energy, must be quantized into

$$k \in \frac{2\pi}{L} \left(\mathbb{Z} - \frac{P_{bc}}{2} + \rho \right) \quad (\text{A33})$$

Therefore, if one gradually turns on λ , all the electron levels, which are equally spaced by $\frac{2\pi}{L}$, will be shifted upward together by an amount of $\rho \cdot \frac{2\pi}{L}$. The maximal shift is equal to *half* of the level spacing, and is only achieved when $\lambda \rightarrow \infty$.

Due to our regularization scheme Eq. (A30), we should not bosonize H_1 by directly applying the point-splitting in Eqs. (A23) and (A24), because the latter relies on the order $\lim_{x' \rightarrow x} \lim_{x_c \rightarrow 0^+}$ of taking limits, whereas Eq. (A30) has $|x - x'| \sim x_c$. Nevertheless, we can still formally write

$$H_1 = \lambda' \int dx \delta(x) \partial_x \phi(x) + \lambda'' \frac{2\pi}{L} N = \lambda' \partial_x \phi(x) \Big|_{x=0} + \lambda'' \frac{2\pi}{L} N, \quad (\text{A34})$$

where N counts the fermion number. λ', λ'' can be directly determined by the phase shift ρ at large distances. Importantly, this determination does not depend on the regularization of the δ -potential, which further relates ρ to the potential λ . Suppose we

were using the second regularization scheme, where the point-splitting in Eqs. (A23) and (A24) applies, then there would be $\lambda' = \lambda'' = \rho$ with $\rho = \lambda$ being the phase shift. As the relation between λ' , λ'' and ρ should not depend on the regularization, $\lambda' = \lambda'' = \rho$ must also hold for the first regularization scheme except that now ρ is given by Eq. (A32). One can verify this statement by examining the phase shift and finite-size spectrum. First, viewing ϕ as a classical field, the δ -potential generates a kink $\phi(0^+) - \phi(0^-) = -2\pi\lambda'$ in its solution, corresponding to a phase shift $e^{i2\pi\lambda'}$ in the fermion field, confirming $\lambda' = \rho$ is the phase shift. Second, according to the discussion above Eq. (A26), the finite-size ground-state energy with a phase shift ρ is $\frac{2\pi}{L} \frac{N(N+1+2\rho-P_{bc})}{2}$, which is changed by $\frac{2\pi}{L} N\rho$ compared to the un-shifted spectrum. This confirms $\lambda'' = \rho$. Therefore, in the first regularization scheme there must be

$$\lambda' = \lambda'' = \rho = \frac{1}{\pi} \arctan(\lambda\pi). \quad (\text{A35})$$

Readers may refer to Ref. [100, 105]) for further discussions.

Gauge transformation canceling the δ -potential—Due to the above discussions, $H_0 + H_1$ can be readily diagonalized in the original fermion representation, with eigenstates $|G\rangle$ given by the phase-shifted fermion spectrum. Now we show that, one can also apply a gauge transformation $U = e^{i\rho\phi(0)}$, where $\phi(0)$ is the bosonized field (see Eq. (A6)), so that $\bar{H} = U H U^\dagger$ reduces to a free Hamiltonian without phase shift. The eigenstates of H in the original representation will thus be given by $|G\rangle = U^\dagger |\bar{G}\rangle$, where $|\bar{G}\rangle$ is the eigenstate of the free-fermion (free-boson) Hamiltonian $\bar{H}$.

By applying the formula

$$e^A \cdot B \cdot e^{-A} = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \dots \quad (\text{A36})$$

and Eq. (A16), we obtain

$$U \phi(x) U^\dagger = \phi(x) - \pi\rho \cdot \text{sgn}_{x_c}(x) + \frac{2\pi\rho}{L} x \quad (\text{A37})$$

$$U \psi(x) U^\dagger = \psi(x) e^{i\pi\rho \cdot \text{sgn}_{x_c}(x)} e^{-i\frac{2\pi\rho}{L} x} \quad (\text{A38})$$

$$U \partial_x \phi(x) U^\dagger = \partial_x \phi(x) - 2\pi\rho \cdot \delta_{x_c}(x) + \frac{2\pi\rho}{L} \quad (\text{A39})$$

Applying this gauge transformation to the kinetic energy term $\frac{1}{4\pi} \int dx : (\partial_x \phi)^2 :$ generates a δ -potential term of the form $-\rho \int dx \delta_{x_c}(x) \partial_x \phi(x)$, which can be used to cancel the coupling Hamiltonian H_1 . Thus, we expect that $U(H_0 + H_1)U^\dagger$ is a free theory.

However, as the finite-size spectrum is of concern, one cannot naively apply the gauge transformation (Eq. (A39)) in real space, which, as well as the commutator Eq. (A16), are derived by taking the $L \rightarrow \infty$ limit before $x_c \rightarrow 0^+$. As explained in Ref. [101] (see discussions around its Eq. (45)), the two limits do not commute. To obtain the *exact* form of $U(H_0 + H_1)U^\dagger$, we work in momentum space and keep its *exact* dependencies on x_c and L until the end. Since

$$\phi(0) = \sum_{q>0} -\sqrt{\frac{2\pi}{qL}} (b(q) + b^\dagger(q)) e^{-x_c q/2}, \quad [\phi(0), b(q)] = \sqrt{\frac{2\pi}{qL}} e^{-x_c q/2}, \quad (\text{A40})$$

Eq. (A36) implies the *exact* transformation

$$U b(q) U^\dagger = b(q) + i\rho \sqrt{\frac{2\pi}{qL}} e^{-\frac{x_c q}{2}}. \quad (\text{A41})$$

It follows

$$\begin{aligned} U \left(\sum_q q b^\dagger(q) b(q) \right) U^\dagger &= \sum_q q \left(b^\dagger(q) - i\rho \sqrt{\frac{2\pi}{qL}} e^{-\frac{x_c q}{2}} \right) \left(b(q) + i\rho \sqrt{\frac{2\pi}{qL}} e^{-\frac{x_c q}{2}} \right) \\ &= \sum_{q>0} q b^\dagger(q) b(q) + \left(\rho \sum_{q>0} i q \sqrt{\frac{2\pi}{qL}} b^\dagger(q) e^{-\frac{x_c q}{2}} + \text{H.c.} \right) + \frac{2\pi}{L} \sum_{q>0} \rho^2 e^{-x_c q} \\ &= \sum_{q>0} q b^\dagger(q) b(q) - \rho \partial_x \phi(x) \Big|_{x=0} + \frac{2\pi}{L} \rho^2 \frac{e^{-x_c \frac{2\pi}{L}}}{1 - e^{-x_c \frac{2\pi}{L}}} \\ &= \sum_{q>0} q b^\dagger(q) b(q) - \rho \partial_x \phi(x) \Big|_{x=0} + \frac{\rho^2}{x_c} \left(1 - \frac{\pi}{L} x_c \right) + \frac{2\pi}{L} \mathcal{O}(x_c L^{-1}). \end{aligned} \quad (\text{A42})$$

Since U commutes with the electron number operators N , for H_0 in Eq. (A26) (with $\alpha = 1$), we have

$$UH_0U^\dagger = H_0 - \rho \partial_x \phi(x) \Big|_{x=0} + \frac{\rho^2}{x_c} \left(1 - \frac{\pi}{L} x_c\right) + \mathcal{O}(x_c L^{-2}) \quad (\text{A43})$$

Let $H_1 = \rho \partial_x \phi(x) \Big|_{x=0} + \rho \frac{2\pi}{L} N$ (Eq. (A34)). Then, since

$$[\partial_x \phi(x) \Big|_{x=0}, \phi(0)] = \sum_{q>0} \frac{2\pi}{qL} \left[-iqb(q) + iqb^\dagger(q), b(q) + b^\dagger(q) \right] e^{-x_c q} = -2i \frac{2\pi}{L} \frac{e^{-x_c \frac{2\pi}{L}}}{1 - e^{-x_c \frac{2\pi}{L}}} = -2i \frac{1}{x_c} \left(1 - \frac{\pi}{L} x_c\right) + \mathcal{O}(x_c L^{-2}), \quad (\text{A44})$$

Eq. (A36) leads to

$$UH_1U^\dagger = H_1 - 2 \frac{\rho^2}{x_c} \left(1 - \frac{\pi}{L} x_c\right) + \mathcal{O}(x_c L^{-2}) \quad (\text{A45})$$

To conclude,

$$U(H_0 + H_1)U^\dagger = \sum_{q>0} q b^\dagger(q)b(q) + \frac{2\pi}{L} \frac{N(N+1 - P_{bc})}{2} + \rho \frac{2\pi}{L} N - \frac{\rho^2}{x_c} \left(1 - \frac{\pi}{L} x_c\right) + \mathcal{O}(x_c L^{-2}). \quad (\text{A46})$$

Eq. (A46) suggests that the ground state energy (for $N = 0$) is changed by $\Delta E = -\frac{\rho^2}{x_c} \left(1 - \frac{\pi}{L} x_c\right)$ due to the δ -potential. The non-divergent energy change is $\frac{\pi}{L} \rho^2$. We can reproduce this result from the fermion side using a much simpler argument. Consider the potential $H_1 = 2\pi\rho \cdot \int dx \delta(x) : \psi^\dagger(x)\psi(x) :$ with the second regularization such that it generates the correct phase shift $\rho \in (-\frac{1}{2}, \frac{1}{2})$. At the single-particle level, ρ shifts the level $k = \frac{2\pi}{L}(n - \frac{P_{bc}}{2})$ to $k = \frac{2\pi}{L}(n + \rho - \frac{P_{bc}}{2})$, where $n \in \mathbb{Z}$. For simplicity, here we assume ρ does not cause a level crossing, i.e., $\rho < \frac{P_{bc}}{2}$. To sum all the energy levels, we introduce an energy truncation factor $e^{-|k| \frac{L}{2\pi} \alpha}$ ($\alpha \rightarrow 0^+$) for each level:

$$E(\rho) = \frac{2\pi}{L} \sum_{n \leq 0} \left(n + \rho - \frac{P_{bc}}{2} \right) e^{(n + \rho - \frac{P_{bc}}{2})\alpha} \xrightarrow{\alpha \rightarrow 0^+} \frac{2\pi}{L} \left(-\frac{1}{\alpha^2} + \frac{1}{12} + \frac{\rho - P_{bc}/2}{2} + \frac{(\rho - P_{bc}/2)^2}{2} \right) + \mathcal{O}(\alpha) \quad (\text{A47})$$

The energy change due to level-shift is $E(\rho) - E(0) = \frac{2\pi}{L} [\frac{\rho}{2} + \frac{\rho^2 - P_{bc}\rho}{2}]$. Even $E_1(\rho)$ and $E_1(0)$ are individually divergent, the difference is finite. After subtracting the constant

$$2\pi\rho \cdot \langle 0 | \psi^\dagger(0)\psi(0) | 0 \rangle = \frac{2\pi}{L} \rho \sum_{n \leq 0} e^{(n - \frac{P_{bc}}{2})\alpha} = \frac{2\pi}{L} \left(\frac{\rho}{\alpha} + \frac{\rho - \rho \cdot P_{bc}}{2} \right) + \mathcal{O}(\alpha) \quad (\text{A48})$$

due to the normal ordering in H_1 , we obtain the total energy change

$$\Delta E = -\frac{2\pi}{L} \cdot \frac{\rho}{\alpha} + \frac{\pi}{L} \cdot \rho^2. \quad (\text{A49})$$

Its non-divergent part is the same as the exact result.

3. Correlation functions

For a free boson Hamiltonian H_0 , the Green's function of $\phi(x)$ can be directly computed using the mode expansion Eq. (A10). Specifically, we define the time-evolved (imaginary or real-time) boson fields by the free H_0 as $\phi_\alpha(\tau, x) = e^{\tau H_0} \phi_\alpha(x) e^{-\tau H_0}$ and $\phi_\alpha(t, x) = e^{itH_0} \phi_\alpha(x) e^{-itH_0}$, with expansion

$$\phi_\alpha(\tau, x) = \sum_{q>0} -\sqrt{\frac{2\pi}{qL}} \left(e^{-q(ix+\tau)} b_\alpha(q) + e^{q(ix+\tau)} b_\alpha^\dagger(q) \right) e^{-\frac{x_c q}{2}} \quad (\text{A50})$$

$$\phi_\alpha(t, x) = \sum_{q>0} -\sqrt{\frac{2\pi}{qL}} \left(e^{-iq(x+t)} b_\alpha(q) + e^{iq(x+t)} b_\alpha^\dagger(q) \right) e^{-\frac{x_c q}{2}} \quad (\text{A51})$$

Because the bath electrons are left-movers, the time-evolved boson fields only depend on $\tau + ix$ and $i(t + x)$. So will be the correlation functions. It can then be calculated that, at zero temperature, for the free bosonic vacuum $|0\rangle$,

$$\langle \phi(\tau, x) \phi(0, 0) \rangle_0 = \sum_{q>0} \frac{2\pi}{qL} e^{-q(ix+\tau+x_c)} \stackrel{=1)}{=} -\ln \left[1 - e^{-\frac{2\pi}{L}(\tau+ix+x_c)} \right] \stackrel{=2)}{=} -\ln \left[\frac{2\pi}{L}(\tau+ix+x_c) \right] \quad (\text{A52})$$

$$\langle \phi(0, 0) \phi(\tau, x) \rangle_0 = \sum_{q>0} \frac{2\pi}{qL} e^{q(ix+\tau-x_c)} \stackrel{=1)}{=} -\ln \left[1 - e^{-\frac{2\pi}{L}(-(\tau+ix)+x_c)} \right] \stackrel{=2)}{=} -\ln \left[\frac{2\pi}{L}(-(\tau+ix)+x_c) \right] \quad (\text{A53})$$

The same expressions apply to the real-time axis by replacing $\tau \rightarrow it$. Several remarks are associated with the equal marks. 1) The series expansion $-\ln(1-x) = \sum_{n=1}^{\infty} \frac{x^n}{n}$ is convergent only for $-1 \leq |x| < 1$. For the correlation functions that we will consider in this work, namely, the τ -ordered, the t -ordered, and the t -retarded correlation functions, the argument always meets the convergence criterion. 2) The thermodynamic limit $\frac{2\pi}{L}x, \frac{2\pi}{L}t, \frac{2\pi}{L}\tau \rightarrow 0$ is taken and $\mathcal{O}(L^{-2})$ terms are omitted, which will be our main focus in this paper for evaluating the correlation functions.

We tabulate the τ -ordered, t -ordered correlation functions in below, with the divergence at $x, \tau, t \rightarrow 0$ subtracted,

$$\begin{aligned} \langle T_\tau \phi(\tau, x) \phi(0, 0) \rangle_0 - \langle \phi(0, 0)^2 \rangle_0 &= \ln \frac{x_c}{(\tau+ix) \cdot \text{sgn}(\tau) + x_c} \quad (T=0^+) \\ \langle T_t \phi(t, x) \phi(0, 0) \rangle_0 - \langle \phi(0, 0)^2 \rangle_0 &= \ln \frac{x_c}{i(t+x) \cdot \text{sgn}(t) + x_c} \quad (T=0^+). \end{aligned} \quad (\text{A54})$$

Following Ref. [101] (see its Eq. (74) and Appendix H2b), the finite-temperature imaginary time function can also be derived as

$$\langle T_\tau \phi(\tau, x) \phi(0, 0) \rangle_0 - \langle \phi(0, 0)^2 \rangle_0 = \ln \frac{\sin(\pi T x_c)}{\sin[\pi T(\tau+ix) \cdot \text{sgn}(\tau) + \pi T x_c]} \stackrel{x_c \rightarrow 0^+}{=} \ln \frac{\pi T x_c}{\sin[\pi T(\tau+ix) \cdot \text{sgn}(\tau) + \pi T x_c]} \quad (\text{A55})$$

where the limit $L \rightarrow \infty$ is taken first. It is periodic over the interval $\tau \in [-\frac{1}{2T}, \frac{1}{2T}]$. Since it reduces to the zero-temperature result in the $T \rightarrow 0^+$ limit, the two orders of limits

$$\lim_{T \rightarrow 0^+} \lim_{x_c \rightarrow 0^+} \lim_{L \rightarrow \infty}, \quad \lim_{x_c \rightarrow 0^+} \lim_{L \rightarrow \infty} \lim_{T \rightarrow 0^+} \quad (\text{A56})$$

give the same correlation functions.

It is also useful to evaluate various correlation functions of the vertex operators $e^{i\kappa\phi}$. A two-point correlation can be calculated by exponentiating the boson correlation function, due to the following identity,

$$\langle e^{i\kappa\phi(z_2)} e^{-i\kappa\phi(z_1)} \rangle_0 = e^{\kappa^2 (\langle \phi(z_2) \phi(z_1) \rangle_0 - \langle \phi(0)^2 \rangle_0)} \quad (\text{A57})$$

where z_2, z_1 can stand for any type of space-time arguments. This identity can be proven in two steps. First, using the Baker-Hausdorff formula (Eq. (A19)), the left hand side equals to $\langle e^{i\kappa(\phi(z_2)-\phi(z_1))} \rangle_0 \cdot e^{\frac{\kappa^2}{2} [\phi(z_2), \phi(z_1)]}$. Second, we use the identity

$$\langle e^B \rangle_0 = \sum_{n=0,2,4,\dots} \frac{1}{(2n)!} \langle B^{2n} \rangle_0 = e^{\frac{1}{2} \langle B^2 \rangle_0}, \quad (\text{A58})$$

where B is a linear superposition of boson creation and annihilation operators, and we have made use of Wick's theorem $\langle B^{2n} \rangle_0 = \frac{(2n)!}{2^n} \frac{1}{n!} (\langle B^2 \rangle_0)^n$. Then we have $\langle e^{i\kappa(\phi(z_2)-\phi(z_1))} \rangle_0 \cdot e^{\frac{\kappa^2}{2} [\phi(z_2), \phi(z_1)]} = \exp(\kappa^2 \langle \phi(z_2)\phi(z_1) - \phi^2(0) \rangle_0)$.

We tabulate some useful time-ordered correlation functions for future convenience:

$$\begin{aligned} \langle T_\tau e^{i\kappa\phi(\tau, x)} e^{-i\kappa\phi(0, 0)} \rangle_0 &= \left(\frac{\pi T x_c}{\sin[\pi T(\tau+ix) \cdot \text{sgn}(\tau) + \pi T x_c]} \right)^{\kappa^2} \stackrel{T \rightarrow 0^+}{=} \left(\frac{x_c}{(\tau+ix) \cdot \text{sgn}(\tau) + x_c} \right)^{\kappa^2} \\ \langle T_t e^{i\kappa\phi(t, x)} e^{-i\kappa\phi(0, 0)} \rangle_0 &\stackrel{T \rightarrow 0^+}{=} \left(\frac{x_c}{i(t+x) \cdot \text{sgn}(t) + x_c} \right)^{\kappa^2} \\ \langle [e^{i\kappa\phi(t, x)}, e^{-i\kappa\phi(0, 0)}] \rangle_0 &= \left(\frac{\pi T x_c}{\sin[i\pi T(t+x) + \pi T x_c]} \right)^{\kappa^2} - \left(\frac{\pi T x_c}{\sin[-i\pi T(t+x) + \pi T x_c]} \right)^{\kappa^2} \\ &\stackrel{T \rightarrow 0^+}{=} \left(\frac{x_c}{i(t+x) + x_c} \right)^{\kappa^2} - \left(\frac{x_c}{-i(t+x) + x_c} \right)^{\kappa^2} \end{aligned} \quad (\text{A59})$$

The notation $T \xrightarrow{0^+}$ means that we take the $L \rightarrow \infty$ limit first and then $T \rightarrow 0^+$, and the notation $T \xrightarrow{0^+}$ means that we take $T \rightarrow 0^+$ first and then $L \rightarrow \infty$, as specified in Eq. (A56).

$\Delta = \frac{\kappa^2}{2}$ is defined as the *scaling dimension* of the vertex operator $Q(t, x) = e^{i\kappa\phi}$, because upon the rescaling $t = bt'$, $x = bx'$, $Q(t, x) = b^{-\Delta} Q'(t', x')$, the correlation function remains unchanged, i.e., $\langle Q(t, x) Q^\dagger(0, 0) \rangle_0 = b^{-2\Delta} \langle Q'(t', x'), Q'^\dagger(0, 0) \rangle_0$. We dub $[e^{i\kappa\phi}] = \frac{\kappa^2}{2}$, $[x] = [t] = -1$.

More generically, a $2n$ -point correlator is given by

$$\left\langle e^{i\kappa_{2n}\phi(z_{2n})} \dots e^{i\kappa_i\phi(z_i)} \dots e^{i\kappa_1\phi(z_1)} \right\rangle_0 = e^{-\frac{1}{2}(\sum_i \kappa_i)^2 \langle \phi(0)^2 \rangle_0} \cdot e^{-\sum_{i' > i} \kappa_{i'} \kappa_i (\langle \phi(z_{i'}) \phi(z_i) \rangle_0 - \langle \phi(0)^2 \rangle_0)} \quad (\text{A60})$$

Since $e^{-\langle \phi(0)^2 \rangle_0} = \frac{2\pi x_c}{L} \rightarrow 0$, the first factor effectively dictates that the correlation function is non-zero only if $\sum_j \kappa_j = 0$. This is a manifestation of the effective $U(1)$ symmetry $\phi \rightarrow \phi + \text{const}$ in the free boson theory. If we use the imaginary-time and specify the time-ordering as $\tau_{2n} > \dots > \tau_2 > \tau_1$,

$$\begin{aligned} \left\langle T_\tau e^{i\kappa_{2n}\phi(z_{2n})} \dots e^{i\kappa_j\phi(z_j)} \dots e^{i\kappa_1\phi(z_1)} \right\rangle_0 &= \exp \left[- \sum_{i' > i} \kappa_{i'} \kappa_i \ln \left(\frac{\pi T x_c}{\sin [\pi T (z_{i'} - z_i) + \pi T x_c]} \right) \right] \\ &\xrightarrow{0^+} \prod_{i' > i} \exp \left[- \sum_{i' > i} \kappa_{i'} \kappa_i \ln \left(\frac{x_c}{z_{i'} - z_i + x_c} \right) \right], \end{aligned} \quad (\text{A61})$$

where $z_i = \tau_i + ix_i$, provided $\sum_{i=1}^{2n} \kappa_i = 0$. For the same reason explained after Eq. (A55), the $\lim_{T \rightarrow 0^+}$ and $\lim_{L \rightarrow \infty}$ limits commute with each other for general vertex correlation functions. Eq. (A61) will be useful in RG calculations and furnishes the Coulomb gas analog.

The free-fermion correlation function can also be recovered using Eq. (A59):

$$\begin{aligned} G(\tau, x) &= - \frac{\text{sgn}(\tau)}{2\pi x_c} \left\langle T_\tau e^{-i\phi(\tau, x)} e^{i\phi(0, 0)} \right\rangle_0 = - \frac{\text{sgn}(\tau) T}{2 \sin [\pi T (\tau + ix) \cdot \text{sgn}(\tau) + \pi T x_c]} \xrightarrow{0^+} - \frac{1}{2\pi} \cdot \frac{1}{\tau + ix + x_c \text{sgn}(\tau)} \\ G(t, x) &\xrightarrow{0^+} -i \left\langle T_t \psi(t, x) \psi^\dagger(0, 0) \right\rangle_0 = -i \frac{\text{sgn}(t)}{2\pi x_c} \left\langle T_t e^{-i\phi(t, x)} e^{i\phi(0, 0)} \right\rangle_0 = - \frac{i}{2\pi} \cdot \frac{1}{i(t+x) + x_c \text{sgn}(t)} \\ G^R(t, x) &= -i\theta(t) \left\langle \{ \psi(t, x), \psi^\dagger(0, 0) \} \right\rangle_0 \xrightarrow{0^+} -i \frac{\theta(t)}{2\pi} \left(\frac{1}{i(t+x) + x_c} + \frac{1}{-i(t+x) + x_c} \right) = -i\theta(t) \cdot \delta_{x_c}(t+x). \end{aligned} \quad (\text{A62})$$

Note that time-ordering of fermion operators introduces a minus sign when two fermion operators are exchanged, whereas this is not the case for bosonic operators. The overall signs $(-1, -i, -i)$ for the imaginary-time, real-time, and retarded Green's functions follow the standard conventions.

B. The quantum impurity model

1. The Anderson model

We consider an Anderson impurity problem with two spin flavors $s = \uparrow, \downarrow$ and two “valley” flavors $l = \pm$. The electron operators on the impurity are denoted as f_{ls} , and the electron operators in the effective one-dimensional chiral bath (see Sec. A for details) are denoted as $\psi_{ls}(x)$. The 2×2 Pauli matrices regarding l and s will be dubbed as $[\sigma^\mu]_{l,l'}$ and $[\zeta^\nu]_{s,s'}$, respectively, with $\mu, \nu = 0, x, y, z$. In realistic systems such as magic-angle twisted bilayer graphene (MATBG) (see Sec. B 6 for details), this “valley” degree of freedom can either represent two degenerate momentum valleys, or represent two degenerate Wannier orbitals that carry opposite orbital angular momenta (OAM) and the corresponding partial waves in the bath. For both cases, l will eventually become an internal degree of freedom (just as spin), despite that we still refer to it as a “valley” index.

We will assume the impurity model to respect the unitary symmetry group of $[U(1)_c \times SU(2)_s \times D_\infty]/\mathbb{Z}_2$. Here $U(1)_c$ is generated by $\sigma^0 \zeta^0$, $SU(2)_s$ is generated by $\sigma^x \zeta^0, \sigma^y \zeta^0, \sigma^z \zeta^0$, and $\mathbb{Z}_2 = \{\sigma^0 \zeta^0, -\sigma^0 \zeta^0\}$. $D_\infty = U(1)_v \rtimes \mathbb{Z}_2$ is the valley symmetry group, where the $U(1)_v$ charge conservation is generated by $\sigma^z \zeta^0$, while the $\mathbb{Z}_2$ component is generated by an valley-flipping action dubbed as $C_2 = \sigma^x \zeta^0$, which guarantees l and $\bar{l}$ to remain degenerate. Rotations in the dihedral group D_∞ follows the algebra relation $C_2 \cdot e^{i\varphi \sigma^z \zeta^0} \cdot C_2 = e^{-i\varphi \sigma^z \zeta^0}$. Origins of these symmetries in the context of MATBG will be reviewed in Sec. B 6.

The Anderson model is

$$\begin{aligned} H &= H_0 + H_{\text{hyb}} + H_{\text{imp}} \\ H_0 &= \sum_{ls} \sum_k k : d_{ls}^\dagger(k) d_{ls}(k) : \quad H_{\text{hyb}} = \sqrt{2\Delta_0} \sum_{ls} \left(\psi_{ls}^\dagger(0) f_{ls} + h.c. \right) \\ H_{\text{imp}} &= \epsilon_f \hat{N} + U \frac{\hat{N}(\hat{N} - 1)}{2} + H_{\text{AH}} \end{aligned} \quad (\text{B1})$$

Here, $d_{ls}(k)$ form the effective chiral fermion bath reproducing the constant hybridization function Δ_0 , with a Fourier transformation to an auxiliary one-dimensional real space $\psi_{ls}(x)$ defined in Eq. (A3). The one-dimensional space is assumed to be of length L ($L \rightarrow \infty$), with the boundary condition of bath electrons chosen as $\psi(-\frac{L}{2}) = \psi(\frac{L}{2})e^{-i\pi P_{bc}}$, so that the momentum $k \in \frac{2\pi}{L}(\mathbb{Z} - P_{bc}/2)$. The normal-ordering $:\cdots:$ to the bath electrons is defined in Eq. (A2). Due to the $SU(2)_s$ and D_∞ symmetries, the Fermi velocities of all bath flavors are degenerate, and the hybridization must be proportional to $\sigma^0 \tau^0$.

H_{imp} is the impurity Hamiltonian that only involves f electrons, and its eigenstates are summarized in Table II. $\hat{N} = \sum_{ls} f_{ls}^\dagger f_{ls}$ counts the total electron number on the impurity. ϵ_f and U denote the on-site potential and the Hubbard repulsion, respectively, while H_{AH} contains all other symmetry-allowed terms that split the N -electron levels into multiplets. Since bilinear terms other than $\sigma^0 \zeta^0$ (Zeeman splittings) necessarily violate the symmetries, we only discuss quartic interactions in H_{AH} .

To find the most general form of H_{AH} , it suffices to 1) classify all bilinear operators $f_{ls} f_{l's'}$ into irreducible representations (irreps) of the symmetry groups D_∞ and $SU(2)_s$, which we refer to as different scattering channels, and 2) assign independent scattering amplitudes to each channel. Since a common scattering amplitude to all channels can be absorbed to a re-definition of Hubbard U , it is convenient to choose one reference channel, and keep track of the relative differences of other channels.

It suffices to label the irreps of D_∞ and $SU(2)_s$ independently, as the two groups commute. For the valley symmetry group D_∞ , we first define the following operator that counts the total $U(1)_v$ charge,

$$\hat{L}^z = \sum_{ls, l's'} f_{ls}^\dagger [\sigma^z]_{l,l'} [\zeta^0]_{s,s'} f_{l's'} \quad \text{with eigenvalues } L^z \in \mathbb{Z} \quad (\text{B2})$$

Since $C_2 = \sigma^x \zeta^0$ anti-commutes with $\hat{L}^z$, $+L^z$ and $-L^z$ states must be degenerate if $L^z \neq 0$. Such irreps must hence be two-fold degenerate. If $L^z = 0$, on the other hand, then the irrep is non-degenerate. Nevertheless, its C_2 eigenvalue can still have two choices, ± 1 . We dub these two irreps as A_1 and A_2 , respectively, following the notation of general D_n groups. We introduce the notation $L = A_1, A_2, 1, 2, 3, \dots$ to uniquely label the irreps of the D_∞ group. For irreps with $L = 1, 2, 3, \dots$, the two degenerate states will be labeled by $L^z = \pm L$. For the direct product of two irreps of D_∞ , there are the following rules,

$$\begin{aligned} A_1 \otimes A_1 &= A_1 & A_1 \otimes A_2 &= A_2 & A_1 \otimes L &= L & A_2 \otimes L &= L \\ L \otimes L' &= |L - L'| \oplus |L + L'| & L \otimes L &= A_1 \oplus A_2 \oplus 2L \end{aligned} \quad (\text{B3})$$

where $L \neq 0, L' \neq 0$, and $L \neq L'$. Also, note that all irreps of D_∞ are real (hence self-conjugate), testified from the Frobenius-Schur indicator, $\text{FSI}[L] = \int dg \cdot \chi^{(L)}(g^2)$, where $\chi^{(L)}(g)$ is the character of group element g in the irrep L , and $\int dg \cdot 1 = 1$ is the group measure. To be specific, D_∞ consists of two connected components, $U(1)_v$ and $C_2 \cdot U(1)_v$. For the non-degenerate irreps $L = A_1$ and A_2 , $\chi^{(L)}(g^2) = 1$ for all $g \in D_\infty$, hence $\text{FSI}[L] = 1$. For the two-fold degenerate irreps, $L = 1, 2, 3, \dots$,

$\chi^{(L)} \left((e^{i\theta\sigma^z})^2 \right) = 2 \cos(L\theta)$, hence the $U(1)_v$ component contributes zero to the FSI, while as $(C_2 \cdot e^{i\theta\sigma^z})^2 = 1$, hence $\chi^{(L)} \left((C_2 \cdot e^{i\theta\sigma^z})^2 \right) = 2$. After the integral, $\text{FSI}[L] = 1$ as well.

For $SU(2)_s$, we follow the standard notation of $SU(2)$ groups, and define

$$\hat{S}^\nu = \frac{1}{2} \sum_{ls, l's'} f_{ls}^\dagger [\sigma^0]_{l, l'} [\zeta^\nu]_{s, s'} f_{l's'} \quad (\nu = x, y, z) \quad \text{with eigenvalues } S^\nu \in \frac{\mathbb{Z}}{2} \quad (\text{B4})$$

We will also denote $\hat{\mathbf{S}} = (\hat{S}^x, \hat{S}^y, \hat{S}^z)$. The irreps of $SU(2)_s$ are uniquely labeled by the spin quantum number $S \in \frac{\mathbb{Z}_{\geq 0}}{2}$, which is defined from the eigenvalues of $\hat{\mathbf{S}}^2 = \sum_{\nu=x,y,z} (\hat{S}^\nu)^2 = S(S+1)$ in the standard way. The degeneracy of an irrep with spin- S is $2S+1$, where the degenerate states are distinguished by $S^z = -S, \dots, S$. The direct product of two irreps is given by $S \otimes S' = |S-S'| \oplus |S-S'|+1 \oplus \dots \oplus |S+S'|$. All the irreps of $SU(2)_s$ are also self-conjugate (real if S is integer, pseudo-real if half-integer).

The irreps of $[D_\infty \times SU(2)_s]/\mathbb{Z}_2$ are hence labeled by $[L, S]$. All irreps are self-conjugate. The total degeneracy of irrep $[L, S]$ is given by the product of the valley degeneracy with the spin degeneracy,

$$\text{DEG}_{[L,S]} = \begin{cases} 2S+1, & L = A_1, A_2 \\ 4S+2, & L = 1, 2, 3, \dots \end{cases} \quad (\text{B5})$$

The valley degeneracy and spin degeneracy within each irrep, if non-trivial, will be labeled by L^z and S^z , respectively.

It is then direct to classify the bilinear operators $f_{ls} f_{l's'}$ (a six-dimensional Hilbert space due to Pauli exclusion principle) into irreps. To begin with, $f_{+\uparrow} f_{-\uparrow}$ and its $SU(2)_s$ rotations span a spin-triplet, and since $L = 0$, there is no additional valley degeneracy. We term this irrep as a triplet ('T', $[L, S] = [A_2, 1]$), according to its total degeneracy 3. Next, the remaining three states necessarily form spin-singlets, and according to their valley charge, can be further classified into an $L = 2$ doublet ('D', $[L, S] = [2, 0]$) and an $L = 0$ singlet ('S', $[L, S] = [A_1, 0]$). The wave-functions of these scattering channels are summarized in Table II, with expressions identical to those irreps of two-electron states.

We choose the triplet channel as the reference channel. Then the general form of the multiplet splitting reads

$$\begin{aligned} H_{\text{AH}} &= -J_S \frac{f_{+\uparrow}^\dagger f_{-\downarrow}^\dagger - f_{+\downarrow}^\dagger f_{-\uparrow}^\dagger}{\sqrt{2}} \frac{f_{-\downarrow} f_{+\uparrow} - f_{-\uparrow} f_{+\downarrow}}{\sqrt{2}} - J_D \sum_{l=\pm} f_{l\uparrow}^\dagger f_{l\downarrow}^\dagger f_{l\downarrow} f_{l\uparrow} \\ &= -\frac{J_S}{4} \sum_{ll's} f_{ls}^\dagger f_{l\bar{s}}^\dagger f_{l'\bar{s}} f_{l's} - \frac{J_D}{2} \sum_{ls} f_{ls}^\dagger f_{l\bar{s}}^\dagger f_{l\bar{s}} f_{ls} \\ &= -\frac{1}{2} \sum_{ss'} \sum_{l_1 l'_1 l_2 l'_2} f_{l_1 s}^\dagger f_{l'_1 s'}^\dagger \begin{pmatrix} J_D & 0 & 0 & 0 \\ 0 & \frac{J_S}{2} & \frac{J_S}{2} & 0 \\ 0 & \frac{J_S}{2} & \frac{J_S}{2} & 0 \\ 0 & 0 & 0 & J_D \end{pmatrix} f_{l'_2 s'} f_{l_2 s} \end{aligned} \quad (\text{B6})$$

with J_S and J_D being parameters to be determined. In the 3rd line, $(l'l) = (++) , (+-), (-+), (--)$. To see that the 3rd line equals the 2nd line, simply note that the $s = s'$ matrix elements in the 3rd line will be canceled after imposing fermion anti-parity. The $s = \bar{s}'$ elements recover the 2nd line. The 3rd line will be useful in Sec. B 6.

In this paper, we discuss the physics for general $J_{S,D}$ that satisfy $|J_{S,D}| \ll U$. If J_S or J_D is positive, the ground state(s) will be spin-singlet(s), hence we will term the splitting as of the anti-Hund's type; while if both J_S and J_D are negative, we term it as of the Hund's type.

It is also useful to re-organize H_{imp} as

$$\begin{aligned} H_{\text{imp}} &= \epsilon_f \hat{N} + \left(U - \frac{1}{4} J_S \right) \frac{\hat{N}(\hat{N}-1)}{2} + J_S \cdot \hat{\mathbf{S}}_+ \cdot \hat{\mathbf{S}}_- - \left(J_D - \frac{1}{4} J_S \right) \sum_l \hat{N}_{l\uparrow} \hat{N}_{l\downarrow} \\ &= \epsilon_f \hat{N} + \left(U - \frac{1}{4} J_S \right) \frac{\hat{N}(\hat{N}-1)}{2} + J_S \cdot \hat{\mathbf{S}}_+ \cdot \hat{\mathbf{S}}_- - \left(J_D - \frac{1}{4} J_S \right) \frac{\hat{N}^2 + (\hat{L}^z)^2 - 2\hat{N}}{4} \end{aligned} \quad (\text{B7})$$

Here, $\hat{S}_l^\nu = \frac{1}{2} \sum_{ss'} f_{ls}^\dagger [\zeta^\nu]_{s, s'} f_{ls'}$ is the spin operator in valley- l , and $\hat{\mathbf{S}}_l = (\hat{S}_l^x, \hat{S}_l^y, \hat{S}_l^z)$. $\hat{N}_{ls} = f_{ls}^\dagger f_{ls}$ so that $\hat{N} = \sum_{ls} \hat{N}_{ls}$.

In Table II, we tabulate all the eigenstates of H_{imp} , according to the $U(1)_c$ charge N , and the good quantum numbers $[L, S]$ of $[D_\infty \times SU(2)_s]/\mathbb{Z}_2$. Notice that, all the one-electron states are dictated to be degenerate, as they form the $[L, S] = [1, \frac{1}{2}]$ irrep, and so are the three-electron states. Therefore, multiplet splitting only occurs in the two-electron subspace. The eigen-energies can be directly read off from Eq. (B7). To begin with, $\hat{N}$ and $(\hat{L}^z)^2 = L^2$ are already given by good quantum numbers. By

$\hat{N}$	$[L, S]$	DEG $_{[L, S]}$	wave-function	energy of H_{imp}
0	$[A_1, 0]$	1	$ \text{emp}\rangle$	$E_0 = 0$
1	$[1, \frac{1}{2}]$	4	$f_{ls}^\dagger \text{emp}\rangle \quad \forall l, s$	$E_1 = \epsilon_f$
2	$[A_1, 0]$	1	$ S\rangle = \frac{f_{+\uparrow}^\dagger f_{-\downarrow}^\dagger - f_{+\downarrow}^\dagger f_{-\uparrow}^\dagger}{\sqrt{2}} \text{emp}\rangle$	$E_S = 2\epsilon_f + U - J_S$
		2	$ D, 2\rangle = f_{+\uparrow}^\dagger f_{+\downarrow}^\dagger \text{emp}\rangle$ $ D, \bar{2}\rangle = f_{-\uparrow}^\dagger f_{-\downarrow}^\dagger \text{emp}\rangle$	$E_D = 2\epsilon_f + U - J_D$
	$[A_2, 1]$	3	$ T, 1\rangle = f_{+\uparrow}^\dagger f_{-\uparrow}^\dagger \text{emp}\rangle$ $ T, 0\rangle = \frac{f_{+\uparrow}^\dagger f_{-\downarrow}^\dagger + f_{+\downarrow}^\dagger f_{-\uparrow}^\dagger}{\sqrt{2}} \text{emp}\rangle$ $ T, \bar{1}\rangle = f_{+\downarrow}^\dagger f_{-\downarrow}^\dagger \text{emp}\rangle$	$E_T = 2\epsilon_f + U$
3	$[1, \frac{1}{2}]$	4	$\text{sgn}(\bar{s}) \cdot f_{l\bar{s}} \text{full}\rangle \quad \forall l, s$	$E_3 = 3\epsilon_f + 3U - \frac{1}{2}J_S - J_D$
4	$[A_1, 0]$	1	$ \text{full}\rangle = f_{+\uparrow}^\dagger f_{+\downarrow}^\dagger f_{-\uparrow}^\dagger f_{-\downarrow}^\dagger \text{emp}\rangle$	$E_4 = 4\epsilon_f + 6U - J_S - 2J_D$

TABLE II. Multiplet levels, diagonalized from the impurity Hamiltonian H_{imp} Eq. (B7).

writing $J_S \cdot \hat{\mathbf{S}}_+ \cdot \hat{\mathbf{S}}_- = \frac{1}{2} J_S [\hat{\mathbf{S}}^2 - \hat{\mathbf{S}}_+^2 - \hat{\mathbf{S}}_-^2]$, where $\hat{\mathbf{S}} = \sum_{l=\pm} \hat{\mathbf{S}}_l$, we can also conveniently evaluate this term. Concretely, except for the two-electron singlet and triplets, all other states have at least one l with $\hat{\mathbf{S}}_l^2 = 0$, therefore, $J_S \cdot \hat{\mathbf{S}}_+ \cdot \hat{\mathbf{S}}_-$ vanishes. For both the singlet and triplets, $\hat{\mathbf{S}}_+^2 = \hat{\mathbf{S}}_-^2 = \frac{1}{2}(\frac{1}{2} + 1)$, while $\hat{\mathbf{S}}^2 = 0$ for the singlet, and $\hat{\mathbf{S}}^2 = 1(1 + 1)$ for the triplet. Consequently, $J_S \cdot \hat{\mathbf{S}}_+ \cdot \hat{\mathbf{S}}_- = -\frac{3}{4}J_S$ for the singlet, and $J_S \cdot \hat{\mathbf{S}}_+ \cdot \hat{\mathbf{S}}_- = \frac{1}{4}J_S$ for the triplet. Adding up contribution from all terms leads to Table II.

Time-reversal and particle-hole symmetries—The model also commutes with an anti-unitary symmetry C_2T that acts as $(C_2T)f_{ls}(C_2T)^{-1} = f_{ls}$ and $(C_2T)d_{ls}(k)(C_2T)^{-1} = d_{ls}(k)$. It originates from the physical (Kramer’s spinful) time-reversal symmetry, in product with an $SU(2)_s$ rotation and a C_2 action, and is hence made “spinless” and “valley-less”. Its origin in MATBG will also be discussed in Sec. B 6. When represented in the auxiliary chiral bath, it does not reverse the momentum k , and hence when Fouriered to the auxiliary real-space, it will map $(C_2T)\psi_{ls}(x)(C_2T)^{-1} = \psi_{ls}(-x)$. Despite this, we still refer to it as a time-reversal symmetry (TRS).

If $P_{\text{bc}} = 0$ or 1, we can also define a (unitary) charge conjugation $f_{ls} \rightarrow f_{ls}^\dagger$, $f_{ls}^\dagger \rightarrow f_{ls}$, $d_{ls}(k) \rightarrow -d_{ls}^\dagger(-k)$, $d_{ls}^\dagger(k) \rightarrow -d_{ls}(-k)$, which leaves $H_0 + H_{\text{hyb}}$ invariant. It transforms the operators contained in H_{imp} as

$$\hat{N} \rightarrow 4 - \hat{N}, \quad (\hat{S}_l^x, \hat{S}_l^y, \hat{S}_l^z) \rightarrow (-\hat{S}_l^x, \hat{S}_l^y, -\hat{S}_l^z) \quad \hat{L}^z \rightarrow -\hat{L}^z. \quad (\text{B8})$$

Using these relations, we find that H_{imp} is invariant under charge conjugation if ϵ_f is tuned to the particle-hole symmetric point (PHS)

$$\epsilon_f = -\frac{3}{2}U + \frac{1}{4}J_S + \frac{1}{2}J_D \quad (\text{PHS}). \quad (\text{B9})$$

Fully anti-symmetrized form of the local interaction—For later convenience, we fully anti-symmetrize H_{imp} as

$$H_{\text{imp}} = \epsilon_f \hat{N} + \frac{1}{4} \sum_{1234} \Gamma_{1234}^0 f_1^\dagger f_2^\dagger f_3 f_4 \quad (\text{B10})$$

where the Arabic numbers are composite indices, i.e., $1 \equiv (l_1, s_1)$, $2 \equiv (l_2, s_2)$, etc.. We can read the (not fully anti-symmetrized yet) vertex function from Eq. (B7) (more concretely, the U term can be re-written as $\frac{U}{2} \hat{N}(\hat{N} - 1) = \frac{U}{2} \sum_{12} f_1^\dagger f_2^\dagger f_2 f_1$, while the J_S and J_D terms can be more conveniently read from Eq. (B6)) as

$$2U \cdot \delta_{l_1 l_4} \delta_{l_2 l_3} \delta_{s_1 s_4} \delta_{s_2 s_3} - 2J_D \cdot \delta_{l_1 l_2} \delta_{l_2 l_3} \delta_{l_3 l_4} \delta_{s_1 s_4} \delta_{s_2 s_3} - J_S \cdot \delta_{l_1 \bar{l}_2} \delta_{l_3 \bar{l}_4} \delta_{s_1 s_4} \delta_{s_2 s_3} \quad (\text{B11})$$

The fully anti-symmetrized vertex is given by

$$\begin{aligned} \Gamma_{1234}^0 = & \Gamma_U^0 \cdot (\delta_{l_1 l_4} \delta_{l_2 l_3} \delta_{s_1 s_4} \delta_{s_2 s_3} - \delta_{l_2 l_4} \delta_{l_1 l_3} \delta_{s_2 s_4} \delta_{s_1 s_3}) + \Gamma_D^0 \cdot \delta_{l_1 l_2} \delta_{l_2 l_3} \delta_{l_3 l_4} (\delta_{s_1 s_3} \delta_{s_2 s_4} - \delta_{s_1 s_4} \delta_{s_2 s_3}) \\ & + \frac{\Gamma_S^0}{2} \cdot \delta_{l_1 \bar{l}_2} \delta_{l_3 \bar{l}_4} (\delta_{s_1 s_3} \delta_{s_2 s_4} - \delta_{s_1 s_4} \delta_{s_2 s_3}) \end{aligned} \quad (\text{B12})$$

The bare parameters are given by $\Gamma_U^0 = U$, $\Gamma_D^0 = J_D$, $\Gamma_S^0 = J_S$. These parameters may flow under renormalization, but the form of Γ^0 will remain unchanged, as it is already the most general form allowed by the symmetry group.

irrep $[L, S]$	DEG $_{[L,S]}$	basis
$[A_1, 0]$	1	$\sigma^0 \zeta^0$
$[A_2, 0]$	1	$\sigma^z \zeta^0$
$[2, 0]$	2	$\sigma^{x,y} \zeta^0$
$[A_1, 1]$	3	$\sigma^0 \zeta^{x,y,z}$
$[A_2, 1]$	3	$\sigma^z \zeta^{x,y,z}$
$[2, 1]$	6	$\sigma^{x,y} \zeta^{x,y,z}$

TABLE III. Hermitian bilinear bath operators classified into irreps of $[L, S]$.

Eq. (B1) with H_{imp} given by Eq. (B7) (with general J_S and J_D) defines the impurity problem. However, there are several special limits of J_S, J_D , where the symmetry group $U(2)_{c,s} \times D_\infty$ is further enlarged.

The $U(4)$ limit—When $J_D = J_S = 0$, the Anderson model is fully $U(4)$ symmetric, with generators given by $\sigma^\mu \zeta^\nu$ for $\mu, \nu = 0, x, y, z$. No multiplet splitting is allowed to occur. Accordingly, in the fully anti-symmetric vertex, only Γ_U^0 survives, while $\Gamma_S^0 = \Gamma_D^0$ remains 0.

The $[U(2)_{c,s} \times SU(2)_v] / \mathbb{Z}_2$ limit—Here $\mathbb{Z}_2 = \{\sigma^0 \zeta^0, -\sigma^0 \zeta^0\}$. When $J_D = J_S \neq 0$, the doublet and singlet become degenerate, and the valley symmetry group will be promoted to an $SU(2)_v$ group, generated by $\sigma^{x,y,z} \zeta^0$. In particular, the original $C_2 = \sigma^x \zeta^0$ action can be understood as $e^{-i\frac{\pi}{2}\sigma^0 \zeta^0} \cdot e^{i\frac{\pi}{2}\sigma^x \zeta^0}$, a product of a $U(1)_c$ rotation and an $SU(2)_v$ rotation.

We now derive the vertex function in this limit. We denote $\Gamma_J^0 \equiv \Gamma_S^0 = \Gamma_D^0$ and split $\Gamma_U^0 = (\Gamma_U^0 - \frac{1}{2}\Gamma_J^0) + \frac{1}{2}\Gamma_J^0$. Then the vertex function can be written as

$$\begin{aligned} \Gamma_{1234}^0 &= \left(\Gamma_U^0 - \frac{1}{2}\Gamma_J^0 \right) \cdot (\delta_{l_1 l_4} \delta_{l_2 l_3} \delta_{s_1 s_4} \delta_{s_2 s_3} - \delta_{l_2 l_4} \delta_{l_1 l_3} \delta_{s_2 s_4} \delta_{s_1 s_3}) \\ &+ \frac{\Gamma_J^0}{2} \cdot \delta_{s_1 s_4} \delta_{s_2 s_3} (\delta_{l_1 l_4} \delta_{l_2 l_3} - \delta_{l_1 \bar{l}_2} \delta_{l_3 \bar{l}_4} - 2\delta_{l_1 l_2} \delta_{l_3 l_4} \delta_{l_2 l_4}) - \frac{\Gamma_J^0}{2} \cdot \delta_{s_1 s_3} \delta_{s_2 s_4} (\delta_{l_1 l_3} \delta_{l_2 l_4} - \delta_{l_1 \bar{l}_2} \delta_{l_3 \bar{l}_4} - 2\delta_{l_1 l_2} \delta_{l_3 l_4} \delta_{l_2 l_4}) \end{aligned} \quad (\text{B13})$$

To simplify the first term in the second row, we rewrite $\delta_{l_1 l_4} \delta_{l_2 l_3} = \delta_{l_1 l_2} \delta_{l_1 l_4} \delta_{l_2 l_3} + \delta_{l_1 \bar{l}_2} \delta_{l_1 l_4} \delta_{l_2 l_3} = \delta_{l_1 l_2} \delta_{l_1 l_3} \delta_{l_2 l_4} + \delta_{l_1 \bar{l}_2} \delta_{l_3 \bar{l}_4} \delta_{l_2 l_3}$. Then, using $1 - \delta_{l_2 l_3} = \delta_{l_2 \bar{l}_3}$, the Kronecker delta functions involving l -indices become $-\delta_{l_1 l_2} \delta_{l_1 l_3} \delta_{l_2 l_4} - \delta_{l_1 \bar{l}_2} \delta_{l_3 \bar{l}_4} \delta_{l_2 \bar{l}_3} = -\delta_{l_1 l_2} \delta_{l_1 l_3} \delta_{l_2 l_4} - \delta_{l_1 \bar{l}_2} \delta_{l_2 l_4} \delta_{l_1 l_3} = -\delta_{l_1 l_3} \delta_{l_2 l_4}$. Hence, the first term in the second row is proportional to $-\delta_{l_1 l_3} \delta_{l_2 l_4} \delta_{s_1 s_4} \delta_{s_2 s_3}$. The second term in the second row is obtained by permuting the indices 3 and 4. Therefore, the vertex equals to

$$\Gamma_{1234}^0 = \left(\Gamma_U^0 - \frac{1}{2}\Gamma_J^0 \right) \cdot (\delta_{l_1 l_4} \delta_{l_2 l_3} \delta_{s_1 s_4} \delta_{s_2 s_3} - \delta_{l_2 l_4} \delta_{l_1 l_3} \delta_{s_2 s_4} \delta_{s_1 s_3}) + \frac{\Gamma_J^0}{2} \cdot (\delta_{l_1 l_4} \delta_{l_2 l_3} \delta_{s_1 s_3} \delta_{s_2 s_4} - \delta_{l_1 l_3} \delta_{l_2 l_4} \delta_{s_1 s_4} \delta_{s_2 s_3}), \quad (\text{B14})$$

which has the form of the models in Refs. [94, 97]. Comparing the above equation to Eq. (4.1) of Ref. [97], we identify our $\Gamma_U^0 - \frac{1}{2}\Gamma_J^0$ and $\frac{1}{2}\Gamma_J^0$ as Γ_C and $-\Gamma_e$ of Ref. [97], respectively.

The $U(2)_+ \times U(2)_- \rtimes \mathbb{Z}_2$ limit—When $J_S = 0$, the spins in the $l = \pm$ valleys are conserved independently. Since $U(1)_c$ and $U(1)_v$ are also preserved, the charges in the $l = \pm$ valleys are conserved independently as well. We dub the continuous group generated by $\frac{\sigma^0 + l \cdot \sigma^z}{2} \zeta^{0,x,y,z}$ as $U(2)_l$ for $l = \pm$, which is the charge-spin rotation group per valley- l . Note the valley-flipping $\mathbb{Z}_2$ factor (generated by σ_x) is not promoted to a continuous symmetry in this case. We can use the valley quantum number L and two spin quantum numbers S_l for $l = \pm$ to label the irreps of scattering channels or two-electron states. The doublet states ($[L, S] = [2, 0]$) are now denoted as $[L, S_+, S_-] = [2, 0, 0]$. The singlet ($[L, S] = [0, 0]$) and triplet ($[L, S] = [0, 1]$) states now become degenerate, as they can be related by an independent spin rotation in $l = +$ and/or $l = -$. They together form a four-fold degenerate irrep $[L, S_+, S_-] = [0, \frac{1}{2}, \frac{1}{2}]$.

2. The Kondo model

We focus the parameter regime $\epsilon_f \approx -\frac{3}{2}U$, where the low-energy configurations are dominated by two- f -electron states, and the multiplet splitting plays a significant role. To obtain the corresponding low-energy theory, we need to carry out a Schrieffer-Wolff (SW) transformation e^{iS} to integrate out the charge fluctuations on the f -impurity that cost $\mathcal{O}(U)$ energies, resulting in an effective Kondo model. For later use, we sketch the formal procedures.

1) Organize the Hilbert space into the low-energy subspace, which contains exactly two f -electrons, and the high-energy subspace, which contains 0, 1, 3 or 4 f -electrons. The projectors to the two subspaces are denoted as $\mathbb{P}_2$ and $1 - \mathbb{P}_2 = \mathbb{P}_0 + \mathbb{P}_1 + \mathbb{P}_3 + \mathbb{P}_4$, respectively. The subscripts indicate the f -electron numbers. We may further divide $\mathbb{P}_2 = \mathbb{P}_S + \mathbb{P}_D + \mathbb{P}_T$, where $\mathbb{P}_S = |S\rangle\langle S|$, $\mathbb{P}_D = \sum_{L^z=2,\bar{2}} |D, L^z\rangle\langle D, L^z|$, and $\mathbb{P}_T = \sum_{S^z=1,0,\bar{1}} |T, S^z\rangle\langle T, S^z|$. $H_0 + H_{\text{imp}}$ is already diagonal in the $\mathbb{P}_2$ and $1 - \mathbb{P}_2$ subspaces, while H_{hyb} induces off-diagonal elements between $\mathbb{P}_2$ and $\mathbb{P}_3$ and between $\mathbb{P}_2$ and $\mathbb{P}_1$. The energy “gap” between the two subspaces is $\mathcal{O}(U)$, while the off-diagonal elements are $\mathcal{O}(\Delta_0)$.

2) To eliminate these off-diagonal elements (perturbatively, in powers of $\frac{\Delta_0}{U}$), we devise such a Hermitian operator $S = \sum_{n=1}^{\infty} S^{(n)}$, where $S^{(n)}$ is of order $\mathcal{O}((\frac{\Delta_0}{U})^n)$. If further assuming that U is much larger than the bath electron band width, the leading order $S^{(1)}$ takes the form of

$$S^{(1)} = \left(\sum_{\Gamma=S,D,T} A_{\Gamma} \cdot \mathbb{P}_3 \left(\sum_{ls} f_{ls}^{\dagger} \psi_{ls}(0) \right) \mathbb{P}_{\Gamma} + \sum_{\Gamma=S,D,T} B_{\Gamma} \cdot \mathbb{P}_1 \left(\sum_{ls} \psi_{ls}^{\dagger}(0) f_{ls} \right) \mathbb{P}_{\Gamma} \right) + \text{H.c.} \quad (\text{B15})$$

where A_{Γ}, B_{Γ} are of order $\mathcal{O}(\frac{\Delta_0}{U})$ and to be determined. e^{iS} serves as a slight unitary rotation between the low- and high-energy subspaces.

3) Compute $\tilde{H} = e^{iS} H e^{-iS} = H + [iS, H] + \frac{1}{2}[iS, [iS, H]] + \dots$ and express each term using the *original* f and ψ operators. Unknown parameters in S are determined by requiring that off-diagonal elements vanish, namely, $(1 - \mathbb{P}_2)\tilde{H}\mathbb{P}_2 = 0$. At the leading order $\mathcal{O}(\Delta_0)$, this implies that $(1 - \mathbb{P}_2)(H_{\text{hyb}} + [iS^{(1)}, H_0 + H_{\text{imp}}])\mathbb{P}_2 = 0$, which fixes A_{Γ} and B_{Γ} . Here, $\mathbb{P}_2$ is still defined according to the particle number of f -operators; however, after the gauge transformation, this f -operator does *not* annihilate a physical electron. Instead, the physical electron operator reads $\tilde{f} = e^{iS} f e^{-iS} = f + [iS^{(1)}, f] + \mathcal{O}((\frac{\Delta_0}{U})^2)$. We will discuss this aspect in more detail in Sec. B 5.

4) As $\tilde{H}$ is now diagonal in the $\mathbb{P}_2$ and $1 - \mathbb{P}_2$ subspaces, we simply keep the low-energy one, $\mathbb{P}_2 \tilde{H} \mathbb{P}_2$. At the leading order $\mathcal{O}(\frac{\Delta_0^2}{U})$, we obtain the Kondo Hamiltonian as $H_K = \frac{i}{2} \mathbb{P}_2 [S^{(1)}, H_{\text{hyb}}] \mathbb{P}_2$. In general, H_K may contain a term that only acts on the impurity; however, this term can be absorbed as a slight shift to the multiplet energies, $E_{\Gamma} \rightarrow E_{\Gamma} + \delta E_{\Gamma}$, which are free parameters to begin with. We therefore neglect it. Remaining terms in H_K will be a coupling between a bilinear operator of bath electrons, and an impurity operator, namely, the Kondo coupling.

U(4) symmetric Kondo model—The SW transformation carried out for the U(4) symmetric case can be found in previous work [53]. We review the result concisely here. H_K contains an SU(4) moment-moment interaction ζ (anti-ferromagnetic, $\zeta > 0$), and a density-density interaction γ ,

$$H_K = (2\pi\zeta) \cdot \sum_{\mu\nu \neq 00} \Theta^{\mu\nu} \cdot \psi^{\dagger} \sigma^{\mu} \zeta^{\nu} \psi + (2\pi\gamma) \cdot \mathbb{P}_2 \cdot : \psi^{\dagger} \sigma^0 \zeta^0 \psi : \quad (\text{B16})$$

Here, we have defined the representation of the SU(4) generators on the 6 two-electron states as

$$\Theta^{\mu\nu} = \mathbb{P}_2 \frac{f^{\dagger} \sigma^{\mu} \zeta^{\nu} f}{2} \mathbb{P}_2 \quad \mu\nu \neq 00 \quad (\text{B17})$$

and abbreviated $\psi^{\dagger} \sigma^{\mu} \zeta^{\nu} \psi = \sum_{ls, l's'} \psi_{ls}^{\dagger}(0) [\sigma^{\mu}]_{ll'} [\zeta^{\nu}]_{ss'} \psi_{l's'}(0)$. If not specified, bath operators in this section all live at $x = 0$. ζ will grow under renormalization, and the system will flow to a Kondo Fermi liquid, where the impurity SU(4) moment gets exactly screened by another SU(4) moment in the bath. Remaining bath electrons sees a $\frac{\pi}{2}$ phase shift at the origin.

General Kondo couplings with $[\text{SU}(2)_s \times D_{\infty}]/\mathbb{Z}_2$ and C_2T symmetries—We now show that, compared to Eq. (B16), the lower symmetry in the general impurity model simply leads to an “anisotropy” in the SU(4) moment-moment couplings ζ , characterized by 5 independent real-valued parameters, as well as allowing the density-density coupling to $\mathbb{P}_S, \mathbb{P}_D$, and $\mathbb{P}_T$ manifolds to be independent. No ‘new’ terms are additionally brought about. The result is summarized in Table IV.

For this sake, a symmetry analysis suffices. As H_K must be Hermitian, it suffices to separately check the Hermitian impurity operators and the Hermitian bilinear bath operators, and classify them into irreps labeled by $[L, S]$. According to the discussions around Eq. (B3), if and only if the impurity operators and the bath operators span the same irrep, their tensor product contains an identity irrep ($[A_1, 0]$) that remains invariant under $[D_{\infty} \times \text{SU}(2)_s]/\mathbb{Z}_2$. Finally, imposing C_2T further rules out some choices.

For the Hermitian bilinear bath operators $\psi_{ls}^{\dagger} \psi_{l's'}$, which span a $4^2 = 16$ dimensional Hilbert space, the decomposition is direct. As both $\psi_{ls}^{\dagger}$ and $\psi_{l's'}$ spans the $[1, \frac{1}{2}]$ irrep (all the irreps of $[D_{\infty} \times \text{SU}(2)_s]/\mathbb{Z}_2$ are self-conjugate, so we do not need to distinguish the irreps of ‘bras’ from ‘kets’, see Sec. B 1), the valley part follows $1 \otimes 1 = A_1 \oplus A_2 \oplus 2$ (see Eq. (B3)), while the spin part follows $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$. The basis operators spanning each irrep are tabulated in Table III. Crucially, each irrep appears just for once.

For the impurity operators $|\Xi\rangle\langle\Xi'|$, they span a $6^2 = 36$ dimensional Hilbert space. Both $|\Xi\rangle$ and $\langle\Xi'|$ span a reducible representation $[A_1, 0] \oplus [2, 0] \oplus [A_2, 1]$ (also dubbed as ‘ $S \oplus D \oplus T$ ’, see Table II). To begin with, there are ‘irrep-diagonal’ operators. For the ‘ S ’ manifold, $[A_1, 0] \otimes [A_1, 0] = [A_1, 0]$, and the operator is given by $\mathbb{P}_S$. For the ‘ D ’ manifold, $[2, 0] \otimes [2, 0] = [A_1, 0] \oplus [A_2, 0] \oplus [4, 0]$, where $[A_1, 0]$ is given by $\mathbb{P}_D$, and $[A_2, 0]$ is given by

$$\Theta^{z0} = |D, 2\rangle\langle D, 2| - |D, \bar{2}\rangle\langle D, \bar{2}| \quad (\text{B18})$$

as defined in Eq. (B17). The operators spanning $[4, 0]$ will be dubbed as

$$\Lambda_x = |D, 2\rangle\langle D, \bar{2}| + \text{H.c.} \quad \Lambda_y = -i|D, 2\rangle\langle D, \bar{2}| + \text{H.c.} \quad (\text{B19})$$

which do not belong to Eq. (B17), and cannot find the corresponding bath bilinear operators to enter the Kondo coupling. For the ‘ T ’ manifold, $[A_2, 1] \otimes [A_2, 1] = [A_1, 0] \oplus [A_1, 1] \oplus [A_1, 2]$. The $[A_1, 0]$ irrep is given by $\mathbb{P}_T$, while $[A_1, 1]$ is the spin-1 operators $\Theta^{0x,0y,0z}$ in Eq. (B17). The $[A_1, 2]$ irrep does not belong to Eq. (B17), and does not appear in Kondo coupling as well.

Then, there are ‘irrep-off-diagonal’ operators. Let us take the off-diagonal blocks between S and D manifolds as an example. Since there are two blocks that are Hermitian conjugate to each other, $|S\rangle\langle D, L^z|$ and $|D, L^z\rangle\langle S|$, the irrep $[A_1, 0] \otimes [2, 0] = [2, 0]$ appears twice. We can Hermitize the basis for the two irreps as following. One is

$$\Theta^{x0} = \frac{|S\rangle\langle D, 2| + |S\rangle\langle D, \bar{2}|}{\sqrt{2}} + \text{H.c.} \quad \Theta^{y0} = i \frac{|S\rangle\langle D, 2| - |S\rangle\langle D, \bar{2}|}{\sqrt{2}} + \text{H.c.} \quad (\text{B20})$$

which follows the definition of Eq. (B17), and the other is

$$\Phi^{x0} = i \frac{|S\rangle\langle D, 2| + |S\rangle\langle D, \bar{2}|}{\sqrt{2}} + \text{H.c.} \quad \Phi^{y0} = - \frac{|S\rangle\langle D, 2| - |S\rangle\langle D, \bar{2}|}{\sqrt{2}} + \text{H.c.} \quad (\text{B21})$$

which does not belong to Eq. (B17). It can be directly verified that (as $\text{SU}(2)_s$ actions are all trivial here, they are not listed)

$$e^{i\theta\sigma^z\zeta^0} \cdot (\Theta^{x0}, \Theta^{y0}) \cdot e^{-i\theta\sigma^z\zeta^0} = (\Theta^{x0}, \Theta^{y0}) \begin{pmatrix} \cos(2\theta) & \sin(2\theta) \\ -\sin(2\theta) & \cos(2\theta) \end{pmatrix} \quad C_2 \cdot (\Theta^{x0}, \Theta^{y0}) \cdot C_2 = (\Theta^{x0}, -\Theta^{y0}) \quad (\text{B22})$$

and (Φ^{x0}, Φ^{y0}) and the bath operators $(\sigma^x\zeta^0, \sigma^y\zeta^0)$ transform in the same way. Therefore, the coupling of $(\sigma^x\zeta^0, \sigma^y\zeta^0)$ to $(\Theta^{x0}, \Theta^{y0})$ and (Φ^{x0}, Φ^{y0}) are both allowed by $[D_\infty \times \text{SU}(2)_s]/\mathbb{Z}_2$. However, they transform differently under C_2T : $(C_2T)(\Theta^{x0}, \Theta^{y0})(C_2T)^{-1} = (\Theta^{x0}, -\Theta^{y0})$, while $(C_2T)(\Phi^{x0}, \Phi^{y0})(C_2T)^{-1} = (-\Phi^{x0}, \Phi^{y0})$, while the bath operator behaves as $(C_2T)(\sigma^x\zeta^0, \sigma^y\zeta^0)(C_2T)^{-1} = (\sigma^x\zeta^0, -\sigma^y\zeta^0)$. Therefore, the bath operator can only couple to $\Theta^{x0, y0}$.

The same analysis also applies to the other off-diagonal blocks. Between S and T , there are two $[A_1, 0] \otimes [A_2, 1] = [A_2, 1]$ irreps, while only the one spanned by $\Theta^{zx, zy, zz}$ is allowed by C_2T to couple to the bath $(\sigma^z\zeta^x, \sigma^z\zeta^y, \sigma^z\zeta^z)$. Between D and T , there are two $[2, 0] \otimes [A_2, 1] = [2, 1]$ irreps, while only the one spanned by $\Theta^{xx, xy, xz, yx, yy, yz}$ is allowed by C_2T to couple to the bath $(\sigma^x\zeta^x, \sigma^x\zeta^y, \sigma^x\zeta^z, \sigma^y\zeta^x, \sigma^y\zeta^y, \sigma^y\zeta^z)$.

In sum, compared to the $\text{U}(4)$ symmetric case, no new Kondo coupling terms are allowed to appear due to the $[D_\infty \times \text{SU}(2)_s]/\mathbb{Z}_2$ and C_2T symmetries. There is only ‘anisotropy’ arising in the coupling constants, as summarized in Table IV. In particular, for the moment-moment couplings, since the $\text{SU}(4)$ breaking effect is a perturbation ($J_{S,D} \ll U$, hence $\zeta_{\mu\nu} \sim \frac{\Delta_0^2}{U + \mathcal{O}(J_{S,D})}$ has the same sign as $\frac{\Delta_0^2}{U}$), we can also expect the signs of the coupling constants to follow the $\text{U}(4)$ symmetric case, being anti-ferromagnetic.

Finally, we remark that, at PHS, $:\psi^\dagger\sigma^0\zeta^0\psi:$ acquires a minus sign under charge conjugation, yet $\mathbb{P}_\Gamma$ ($\Gamma = S, D, T$) does not. Therefore, the density-density coupling will be forbidden so that all $\gamma_\Gamma = 0$. Since the density-density coupling is in general not relevant under RG, we will take the advantage of assuming a PHS to ignore it.

Further down-folding the Kondo model— Suppose we are carrying out an RG (for example, a poorman scaling) to this general Kondo model with $H_0 + H_{\text{imp}} + H_K$, where $H_{\text{imp}} = \sum_{\Gamma=S,D,T} E_\Gamma \cdot \mathbb{P}_\Gamma$ (see Table II), and an anti-ferromagnetic H_K given by Table IV. As the charge fluctuation has been integrated out, we are starting with an initial energy scale D satisfying $|J_{S,D}| \ll D \ll U$. Therefore, initially, the multiplet splitting induced by $J_{S,D}$ is not important, and the five independent moment-moment couplings will remain approximately equal as ζ . ζ will grow as D is lowered, similar to the $\text{U}(4)$ symmetric case. If ζ already diverges at some $D_K \gg |J_{S,D}|$ (or equivalently speaking, the system flows to a strong-coupling fixed point, evidenced by *e.g.* the low-energy bath phase shift saturating $\frac{\pi}{2}$), then the system should share the same universal properties as the $\text{U}(4)$ symmetric model. However, if ζ has not diverged when D reaches the scale of multiplet splitting, yet we are still interested in physics with temperature $k_B T \ll D \sim |J_{S,D}|$, then we will have to further down-fold the low-energy Hilbert space.

In Secs. B 3 and B 4, we will discuss the further down-folded models in more detail.

3. The doublet regime and a pair-Kondo model

We now specify to such parameters $U \gg J_D > \max(J_S, 0)$, and assume the Kondo resonance has *not* formed at the energy scale of $D \lesssim J_D$. Then, we can further divide the Hilbert space into a low-energy one $\mathbb{P}_D$ and a high-energy one $\mathbb{P}_2 - \mathbb{P}_D$. In this way, the low-energy block has Hamiltonian $H = H_0 + \mathbb{P}_D H_{\text{imp}} \mathbb{P}_D + \mathbb{P}_D H_K \mathbb{P}_D$, where $\mathbb{P}_D H_{\text{imp}} \mathbb{P}_D$ serves as an energy constant in the entire low-energy space and can be dropped, while (assuming PHS)

$$\mathbb{P}_D H_K \mathbb{P}_D = (2\pi\lambda_z) \cdot \Theta^{z0} \cdot \psi^\dagger \sigma^z \zeta^0 \psi \quad (\text{B23})$$

	irrep	DEG _[L,S]	impurity operator	coupled to bath bilinear operator	coupling constant
Within S	$[A_1, 0]$	1	$\mathbb{P}_S$	$\sigma^0 \zeta^0$	γ_S
Within D	$[A_1, 0]$	1	$\mathbb{P}_D$	$\sigma^0 \zeta^0$	γ_D
	$[A_2, 0]$	1	Θ^{z0}	$\sigma^z \zeta^0$	λ_z
	$[4, 0]$	2	$\Lambda_{x,y}$	—	—
Within T	$[A_1, 0]$	1	$\mathbb{P}_T$	$\sigma^0 \zeta^0$	γ_T
	$[A_1, 1]$	3	$\Theta^{0x,0y,0z}$	$\sigma^0 \zeta^{x,y,z}$	ζ_{0z}
	$[A_1, 2]$	5	$ T, 1\rangle\langle T, \bar{1} $, etc	—	—
Between S, D	$[2, 0]$	2	$\Theta^{x0,y0}$	$\sigma^{x,y} \zeta^0$	ζ_x
Between S, T	$[A_2, 1]$	3	$\Theta^{zx,zy,zz}$	$\sigma^z \zeta^{x,y,z}$	ζ_{zz}
Between D, T	$[2, 1]$	6	$\Theta^{xx,xy,xz,yx,yy,yz}$	$\sigma^{x,y} \zeta^{x,y,z}$	ζ_{xz}

TABLE IV. Kondo couplings that are allowed by the D_∞ , $SU(2)_s$ and C_2T symmetries. We also denote Θ^{z0} as Λ_z . The couplings γ_S , γ_D , γ_T break the particle-hole symmetry and are in general not relevant in the low-energy physics.

namely, the impurity behaves as a local moment with a two-fold valley degeneracy, and it can only couple to a bath bilinear operator in an Ising form. Recall from Sec. B 2 that $\lambda_z > 0$ is anti-ferromagnetic.

Now we carry out another SW transformation to eliminate the high-energy multiplet fluctuations, $(\mathbb{P}_2 - \mathbb{P}_D)H\mathbb{P}_D$, which will lead to new couplings in the low-energy space $\mathbb{P}_D$. As the off-diagonal process $(\mathbb{P}_2 - \mathbb{P}_D)H\mathbb{P}_D$ contains a bilinear bath operator $\psi^\dagger\psi$, the second-order correction to the low-energy space after the SW transformation will be at most quartic in ψ fields, whose general form has not been discussed. From the RG perspective, a quartic bath operator O located at $x = 0$ has an irrelevant (classical) scaling dimension $[\psi^\dagger\psi^\dagger\psi\psi] = 2$, if the quantum correction is not important, and hence can be neglected. However, we find that SW transformation indeed leads to a quartic coupling to $\Lambda_{x,y}$ that has a significant quantum correction with its interplay with λ_z . We obtain its form in below, and bosonize the model. The quartic coupling to Λ_z can be neglected, as the bilinear coupling λ_z already plays an important role in RG. The RG analysis will be presented in Sec. D. We also discuss the quartic coupling to $\mathbb{P}_D$ in Sec. H 2, which serves as an effective interaction at bath $x = 0$, and is confirmed numerically as irrelevant.

In this doublet regime, we will abbreviate $|D, L^z\rangle = |L^z\rangle$ with $L^z = \pm 2$ without causing confusion. Also, we will term $\Lambda_z = \Theta^{z0}$, in order to stress that $\Lambda_{x,y,z}$ form a new set of Pauli matrices. Specifically, we denote

$$\Lambda_z = |2\rangle\langle 2| - |\bar{2}\rangle\langle \bar{2}|, \quad \Lambda_x = |2\rangle\langle \bar{2}| + |\bar{2}\rangle\langle 2|, \quad \Lambda_y = -i|2\rangle\langle \bar{2}| + i|\bar{2}\rangle\langle 2|, \quad \Lambda_+ = |2\rangle\langle \bar{2}|, \quad \Lambda_- = |\bar{2}\rangle\langle 2| \quad (\text{B24})$$

Note that the eigenvalues of $\Lambda_z = \pm 1$ correspond to the $L^z = \pm 2$ states, respectively.

As stated in Sec. B 2, the impurity operators $\Lambda_\pm = \frac{\Lambda_x \pm i\Lambda_y}{2}$ cannot couple to bilinears $\psi_{l's'}^\dagger\psi_{l's}$, because the $U(1)_v$ charge cannot match. Therefore, we search for the quartic couplings. The only terms that match the $U(1)_v$ charge read

$$\lambda_x \cdot |2\rangle\langle \bar{2}| \cdot \psi_{-\downarrow}^\dagger \psi_{-\uparrow}^\dagger \psi_{+\uparrow} \psi_{+\downarrow} + \lambda_x^* \cdot |\bar{2}\rangle\langle 2| \cdot \psi_{+\downarrow}^\dagger \psi_{+\uparrow}^\dagger \psi_{-\uparrow} \psi_{-\downarrow}, \quad (\text{B25})$$

where the second term is hermitian conjugation of the first term. Applying C_2 interchanges the two terms, hence ensuring λ_x is real-valued. Since it must scatter an electron pair (which belongs to the $[2, 0]$ irrep, namely, the doublet ‘ D ’) to flip the impurity, and this term can become relevant and drive a Kondo Fermi liquid under RG, we term it as a pair-Kondo coupling (PK).

Plus H_0 and $\mathbb{P}_D H_K \mathbb{P}_D$ in Eq. (B23), the total effective Hamiltonian in the doublet regime will take the form

$$H_{\text{PK}} = \sum_{lsk} k : d_{ls}^\dagger(k) d_{ls}(k) : + (2\pi\lambda_z) \cdot \Lambda_z \sum_{ls} l \cdot \psi_{ls}^\dagger(0) \psi_{ls}(0) + (2\pi)^2 x_c \lambda_x \left(\Lambda_+ \cdot \psi_{-\downarrow}^\dagger(0) \psi_{-\uparrow}^\dagger(0) \psi_{+\uparrow}(0) \psi_{+\downarrow}(0) + h.c. \right). \quad (\text{B26})$$

Here, x_c is an ultraviolet length scale (Sec. A). It is explicitly introduced here so that both λ_z and λ_x are *dimensionless* variables.

As the result of the second SW transformation, λ_x can be estimated to be of order $\mathcal{O}(\frac{1}{x_c J_D} (\frac{\Delta_0}{U})^2)$. Any correction to λ_z during the SW transformation must be of the same order, and hence can be neglected compared to the original value of $\lambda_z \sim \mathcal{O}(\frac{\Delta_0}{U})$. The sign of λ_x is not important, because it can be flipped after applying a gauge transformation $i\Lambda_z$ to the impurity, while the physics cannot be changed by such a gauge transformation. Therefore, it is the sign of λ_z that determines the physics, which has been shown as anti-ferromagnetic ($\lambda_z > 0$).

Unlike in the conventional Kondo problem, it is difficult to use naive poorman’s scaling to capture the low energy physics of the pair-Kondo model (Eq. (B26)). Consider integrating out all fermion modes between the energies $De^{-\ell}$ and $De^{-\ell-d\ell}$. To first order of $d\ell$, the renormalization to λ_z seems to be zero. The perturbation terms that are proportional to Λ_z are given by

$$\sim \Lambda_x \Lambda_y \cdot \psi^\dagger \psi^\dagger \overline{\psi \psi} \psi^\dagger \psi^\dagger \psi \psi + (\text{other single particle-hole pair contractions}). \quad (\text{B27})$$

They are sixth order terms in the fermion operators and hence cannot contribute to λ_z . In order to obtain renormalization to λ_z , one has to keep the $\lambda'_z \Lambda_z \cdot \psi^\dagger \psi^\dagger \psi^\dagger \psi \psi \psi$ and $\lambda''_z \Lambda_z \cdot \psi^\dagger \psi^\dagger \psi \psi \psi$ terms in the effective Hamiltonian and solve a set of flow equations of $\lambda_z, \lambda_x, \lambda'_z, \lambda''_z$, which complicate the discussions. Another complication comes from the different scaling dimensions of λ_z and λ_x . Given $[x] = -1$, $[\psi] = \frac{1}{2}$, and $[H_{\text{PK}}] = 1$, there must be $[\lambda_z] = 0$, $[\lambda_x] = -1$, suggesting the tree-level flow equation

$$\frac{d\lambda_x}{d\ell} = -\lambda_x + \mathcal{O}(\lambda_{z,x}^2). \quad (\text{B28})$$

The different scaling dimensions are also reflected in the fact that phase volumes in the λ_z and λ_x terms are $\mathcal{O}(D^2 e^{-2\ell})$ and $\mathcal{O}(D^4 e^{-4\ell})$, respectively. These difficulties will be resolved by the bosonization approach.

According to the bosonization dictionary (see Sec. A), H_{PK} is mapped to

$$\begin{aligned} H_{\text{PK}} = & \sum_{ls} \left(\int \frac{dx}{4\pi} : (\partial_x \phi_{ls}(x))^2 : + \frac{2\pi}{L} \frac{N_{ls}(N_{ls} + 1 - P_{\text{bc}})}{2} \right) + \rho_z \Lambda_z \sum_{ls} l \cdot \left(\partial_x \phi_{ls}(x) \Big|_{x=0} + \frac{2\pi}{L} N_{ls} \right) \\ & + \frac{\lambda_x}{x_c} \left(\Lambda_+ \cdot F_{-\downarrow}^\dagger F_{-\uparrow}^\dagger F_{+\uparrow} F_{+\downarrow} \cdot e^{i(\phi_{-\downarrow}(0) + \phi_{-\uparrow}(0) - \phi_{+\uparrow}(0) - \phi_{+\downarrow}(0))} + h.c. \right). \end{aligned} \quad (\text{B29})$$

where N_{ls} is the bath electron number measured from the normal-ordering reference state, and $\phi_{ls}(x)$ and F_{ls} are the boson field and Klein factor corresponding to $\psi_{ls}(x)$, respectively.

$$\rho_z = \frac{\arctan \pi \lambda_z}{\pi} \in \left(-\frac{1}{2}, \frac{1}{2} \right) \quad (\text{B30})$$

is the phase shift caused by λ_z . One may refer to discussions around Eqs. (A26) and (A34) for the bosonizations for kinetic Hamiltonian and the λ_z -coupling Hamiltonian, respectively. The term $\int \frac{dx}{4\pi} : (\partial_x \phi_{ls})^2 :$ can be equivalently written as $\sum_{q>0} q : b_{ls}^\dagger(q) b_{ls}(q) :$. Bosonization of the λ_x -coupling term is obtained by a straightforward substitution of the identity Eq. (A6).

To further simplify the problem, we introduce the flavor charges,

$$\begin{pmatrix} N_c \\ N_v \\ N_s \\ N_{vs} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} N_{+\uparrow} \\ N_{+\downarrow} \\ N_{-\uparrow} \\ N_{-\downarrow} \end{pmatrix}, \quad \text{written compactly as} \quad N_\chi = \sum_{ls} R_{\chi;ls} N_{ls} \quad (\text{B31})$$

By these definitions, N_χ must take values in $\frac{\mathbb{Z}}{2}$. However, not all values of $N_\chi \in \frac{\mathbb{Z}}{2}$ are physical, because after transforming back to the N_{ls} basis, they may not correspond to integer-valued N_{ls} .

The four $N_\chi \in \frac{\mathbb{Z}}{2}$ are physical, i.e., corresponding to integer N_{ls} , iff they satisfy the following three conditions

$$\begin{aligned} 2N_c = 2N_s = 2N_v = 2N_{vs} \mod 2, \\ N_c + N_v = N_s + N_{vs} \mod 2, \quad N_c - N_v = N_s - N_{vs} \mod 2. \end{aligned} \quad (\text{B32})$$

These conditions are referred to as *free-gluing conditions* [103]. It is direct to show that they are necessary conditions for physical N_χ . Starting from the vacuum where $N_\chi = 0$, every additional electron in the four flavors $\{l = \pm, s = \uparrow\downarrow\}$ changes the parity of all $2N_\chi$ simultaneously, verifying the first condition. The second and third conditions in Eq. (B32) are equivalent to $N_{l\downarrow} \in \mathbb{Z}$ for $l = +$ and $-$, respectively. Conditions in Eq. (B32) are also sufficient to guarantee integer N_{ls} . There must be $N_{l\downarrow} \in \mathbb{Z}$ ($\eta = \pm$) given the second and third conditions. To show that $N_{l\uparrow} \in \mathbb{Z}$ as well, we revisit the first condition, which dictates $2N_c + l \cdot 2N_v = 2N_{l\uparrow} + 2N_{l\downarrow} = 0 \mod 2$, namely, $N_{l\uparrow} + N_{l\downarrow} \in \mathbb{Z}$. Since $N_{l\downarrow} \in \mathbb{Z}$, there must also be $N_{l\uparrow} \in \mathbb{Z}$. Therefore, any four N_χ that satisfy Eq. (B32) correspond to integer N_{ls} and hence are physical.

Since $[N_v, F_{ls}] = -\frac{l}{2} F_{ls}$ ($l = \pm$), the following U(1) charges are conserved in the presence of λ_x :

$$N_c, \quad N_s, \quad N_{vs}, \quad N_v^{(\text{tot})} = N_v + \Lambda_z. \quad (\text{B33})$$

We introduce the boson fields corresponding to the U(1) charges:

$$\phi_\chi(x) = \sum_{ls} R_{\chi;ls} \phi_{ls}(x), \quad \chi = c, v, s, vs \quad (\text{B34})$$

which is a unitary transformation to the boson fields and preserves the canonical commutation relations. Correspondingly, we also define the $b_\chi(q)$ components. We now rewrite H_{PK} (Eq. (B26)) as

$$\begin{aligned} H_{\text{PK}} = & \sum_\chi \left(\int \frac{dx}{4\pi} : (\partial_x \phi_\chi(x))^2 : + \frac{2\pi}{L} \cdot \frac{N_\chi^2}{2} \right) + \frac{2\pi}{L} N_c (1 - P_{\text{bc}}) + 2\rho_z \Lambda_z \left(\partial_x \phi_v(x) \Big|_{x=0} + \frac{2\pi}{L} N_v \right) \\ & + \frac{\lambda_x}{x_c} \left(\Lambda_+ F_v \cdot e^{-2i\phi_v(0)} + \Lambda_- F_v^\dagger \cdot e^{2i\phi_v(0)} \right), \end{aligned} \quad (\text{B35})$$

where

$$F_v = F_{-\downarrow}^\dagger F_{-\uparrow}^\dagger F_{+\uparrow} F_{+\downarrow}. \quad (\text{B36})$$

The term $\int \frac{dx}{4\pi} : (\partial_x \phi_\chi)^2 :$ can be equivalently written as $\sum_{q>0} q b_\chi^\dagger(q) b_\chi(q)$. We find that the impurity only couples to the valley fluctuation ϕ_v , whereas other channels are decoupled from the local impurity.

Eq. (B35) can be further simplified by the unitary transformation $U = e^{2i\rho_z \Lambda_z \phi_v(0)}$. ρ_z will be absorbed by a phase jump in the transformed Hamiltonian $\bar{H}_{\text{PK}} = U H_{\text{PK}} U^\dagger$. (Hereafter we always denote $\bar{O} = U O U^\dagger$ for any operator O .) Following the calculations around Eq. (A46), we find the first row of Eq. (B35) is transformed to

$$\sum_\chi \left(\int \frac{dx}{4\pi} : (\partial_x \phi_\chi(x))^2 : + \frac{2\pi}{L} \cdot \frac{N_\chi^2}{2} \right) + \frac{2\pi}{L} N_c (1 - P_{\text{bc}}) + \frac{2\pi}{L} \cdot 2\rho_z \Lambda_z N_v - \frac{4\rho_z^2}{x_c} \left(1 - \frac{\pi}{L} x_c \right). \quad (\text{B37})$$

To derive the transformation of the second row, we notice

$$U \Lambda_+ U^\dagger = \sum_n \frac{(2i\rho_z \phi_v(0))^n}{n!} [\Lambda_z^{(n)}, \Lambda_+] = \Lambda_+ \sum_n \frac{(4i\rho_z \phi_v(0))^n}{n!} = \Lambda_+ e^{4i\rho_z \phi_v(0)}, \quad (\text{B38})$$

where we have made use of $[\Lambda_z, \Lambda_+] = 2\Lambda_+$. In summary, we have

$$\begin{aligned} \bar{H}_{\text{PK}} = & \sum_\chi \left(\int \frac{dx}{4\pi} : (\partial_x \phi_\chi(x))^2 : + \frac{2\pi}{L} \cdot \frac{N_\chi^2}{2} \right) + \frac{2\pi}{L} N_c (1 - P_{\text{bc}}) + \frac{2\pi}{L} \cdot 2\rho_z \Lambda_z N_v - \frac{4\rho_z^2}{x_c} \left(1 - \frac{\pi}{L} x_c \right) \\ & + \frac{\lambda_x}{x_c} \left(\Lambda_+ F_v \cdot e^{-2i(1-2\rho_z)\phi_v(0)} + \Lambda_- F_v^\dagger \cdot e^{2i(1-2\rho_z)\phi_v(0)} \right). \end{aligned} \quad (\text{B39})$$

The term $\int \frac{dx}{4\pi} : (\partial_x \phi_\chi)^2 :$ can be equivalently written as $\sum_{q>0} q b_\chi^\dagger(q) b_\chi(q)$. This model has two solvable fixed points: When $\lambda_x = 0$, it is diagonalized by the quantum numbers $n_\chi(q) = b_\chi^\dagger(q) b_\chi(q)$, N_χ , Λ_z . When $\rho_z = \rho_z^* = \frac{1}{4}$, $e^{-2i(1-2\rho_z^*)\phi_v(0)} = e^{-i\phi_v(0)}$ has the scaling dimension of a fermion field (Eq. (A59)) and the operator $F_v \cdot e^{-i\phi_v(0)}$ can be mapped to a pseudo fermion. Then the Hamiltonian is almost equivalent to a free-fermion problem.

4. The local singlet regime

We now specify to such parameters $U \gg J_S \geq J_D > 0$, and derive the effective Hamiltonian within the low-energy space including $\mathbb{P}_S + \mathbb{P}_D$. The aim of the Hamiltonian is to investigate the RG flow near the phase transition between the Kondo Fermi liquid (FL) and the local singlet phase (LS), which will be presented in Sec. F.

For this purpose, let us assume the Kondo resonance has *not* formed at the energy scale of $D \lesssim J_S$. The corresponding low-energy space will be $\mathbb{P}_S + \mathbb{P}_D$, while the high-energy space is given by $\mathbb{P}_T$. We first write down the Hamiltonian in the low-energy block (also utilizing PHS)

$$\begin{aligned} H^{(S,D)} &= H_0 + (\mathbb{P}_S + \mathbb{P}_D)(H_{\text{imp}} + H_K)(\mathbb{P}_S + \mathbb{P}_D) \\ (\mathbb{P}_S + \mathbb{P}_D)H_{\text{imp}}(\mathbb{P}_S + \mathbb{P}_D) &= J \cdot \mathbb{P}_D + \text{const} \quad \text{where } J = J_S - J_D \geq 0 \\ (\mathbb{P}_S + \mathbb{P}_D)H_K(\mathbb{P}_S + \mathbb{P}_D) &= (2\pi\lambda_z) \cdot \Theta^{z0} \cdot \psi^\dagger \sigma^z \zeta^0 \psi + (2\pi \frac{\zeta_x}{\sqrt{2}}) \cdot \left(\Theta^{x0} \cdot \psi^\dagger \sigma^x \zeta^0 \psi + \Theta^{y0} \cdot \psi^\dagger \sigma^y \zeta^0 \psi \right) \end{aligned} \quad (\text{B40})$$

In principle, we still need to apply a second SW transformation to eliminate the off-diagonal elements $(\mathbb{P}_S + \mathbb{P}_D)H\mathbb{P}_T$, which can induce quartic terms, including the pair-Kondo term λ_x introduced in Sec. B3, and terms like $\mathbb{P}_S \cdot \psi^\dagger \psi^\dagger \psi \psi$, etc. However, as the Kondo-LS transition will be governed by the interplay between λ_z, ζ_x, J (to be shown in Sec. F), while these quartic terms are in general more irrelevant, it suffices to discard them in the RG analysis. We also mention that, as the bilinear couplings and the impurity Hamiltonian are already at their most general form, any corrections arising from the second SW transformation can be simply absorbed as a re-definition to λ_z, ζ_x , or J . Therefore, H in Eq. (B40) is the total effective Hamiltonian that we will consider.

Now we introduce more convenient symbols, and bosonize Eq. (B40). We abbreviate $|D, L^z\rangle = |L^z\rangle$ for $L^z = 2, \bar{2}$, and abbreviate $|S\rangle = |0\rangle$, to stress that they are linked by varying the $U(1)_v$ charge. We will also denote

$$\Lambda_z = |2\rangle\langle 2| - |\bar{2}\rangle\langle \bar{2}| = \Theta^{z0} \quad \Theta_+ = |2\rangle\langle 0| + |0\rangle\langle \bar{2}| = \frac{\Theta^{x0} + i\Theta^{y0}}{\sqrt{2}} \quad \Theta_- = |0\rangle\langle 2| + |\bar{2}\rangle\langle 0| = \frac{\Theta^{x0} - i\Theta^{y0}}{\sqrt{2}} \quad (\text{B41})$$

Notice that $\mathbb{P}_D = \Lambda_z^2$, $\Lambda_+ = \Theta_+^2$. With these notations, we re-write the Hamiltonian and bosonize it following Sec. A:

$$\begin{aligned}
 H^{(S,D)} &= \sum_{ls} k : d_{ls}^\dagger(k) d_{ls}(k) : + J \cdot \Lambda_z^2 + (2\pi\lambda_z)\Lambda_z \sum_{ls} l : \psi_{ls}^\dagger(0) \psi_{ls}(0) + (2\pi\zeta_x) \left(\Theta_+ \cdot \sum_s \psi_{-s}^\dagger(0) \psi_{+s}(0) + h.c. \right) \\
 &= \sum_{ls} \int \frac{dx}{4\pi} : (\partial_x \phi_{ls}(x))^2 : + J \cdot \Lambda_z^2 + \rho_z \Lambda_z \sum_{ls} l : (\partial_x \phi_{ls}(0)) : + \frac{\zeta_x}{x_c} \left(\Theta_+ \cdot \sum_s F_{-s}^\dagger F_{+s} e^{i(\phi_{-s}(0) - \phi_{+s}(0))} + h.c. \right)
 \end{aligned} \tag{B42}$$

Here, we ignore the finite-size terms of $\mathcal{O}(\frac{2\pi}{L})$, as they should not affect the RG flow.

For later convenience, we introduce the following basis,

$$\begin{pmatrix} \phi_c \\ \phi_s \\ \varphi_\uparrow \\ \varphi_\downarrow \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \phi_{+\uparrow} \\ \phi_{+\downarrow} \\ \phi_{-\uparrow} \\ \phi_{-\downarrow} \end{pmatrix} \tag{B43}$$

where φ_s for $s = \uparrow, \downarrow$ are superpositions of ϕ_v and ϕ_{vs} (see Eq. (B34)), hence correspond to the valley fluctuations per spin sector. They should not be confused with the spin fluctuation ϕ_s . We also define the composite Klein factors $F_s = F_{-s}^\dagger F_{+s}$ for $s = \uparrow, \downarrow$, which correspond to the valley charge variation per spin sector. Using the fact that F_{ls} anti-commutes with $F_{l's'}^\dagger$ for $ls \neq l's'$, there is $F_\uparrow F_\downarrow = F_v$ (see Eq. (B36)).

With these notations, we arrive at the effective Hamiltonian

$$\begin{aligned}
 H &= \int \frac{dx}{4\pi} \left(: (\partial_x \phi_c(x))^2 : + : (\partial_x \phi_s(x))^2 : + \sum_s : (\partial_x \varphi_s(x))^2 : \right) + J \cdot \Lambda_z^2 + \rho_z \Lambda_z \sqrt{2} \sum_s : (\partial_x \varphi_s(0)) : \\
 &\quad + \frac{\zeta_x}{x_c} \cdot \left(\Theta_+ \sum_s F_s \cdot e^{-i\sqrt{2}\varphi_s(0)} + h.c. \right)
 \end{aligned} \tag{B44}$$

Similar to Sec. B3, the ρ_z coupling can be absorbed by a gauge transformation $U = e^{i\sqrt{2}\rho_z\Lambda_z\varphi_\uparrow(0) + i\sqrt{2}\rho_z\Lambda_z\varphi_\downarrow(0)}$. Let us denote the transformed Hamiltonian as $\bar{H} = U H U^\dagger$, and divide $\bar{H} = \bar{H}_0 + \bar{H}_x$. Here, $\bar{H}_0$ can be calculated following calculations around Eq. (A46),

$$\begin{aligned}
 \bar{H}_0 &= U \left(\sum_{s=\uparrow\downarrow} \int \frac{dx}{4\pi} : (\partial_x \varphi_s)^2 : + J \cdot \Lambda_z^2 + \sqrt{2}\rho_z\Lambda_z \cdot \sum_s \partial_x \varphi_s(x) \Big|_{x=0} \right) U^\dagger \\
 &= \sum_{s=\uparrow\downarrow} \int \frac{dx}{4\pi} : (\partial_x \varphi_s)^2 : + \left(J - \frac{4\rho_z^2}{x_c} \right) \cdot \Lambda_z^2
 \end{aligned} \tag{B45}$$

while due to $[\Lambda_z, \Theta_+] = \Theta_+$, there is $U\Theta_\pm U^\dagger = e^{\pm i\sqrt{2}\rho_z(\varphi_\uparrow(0) + \varphi_\downarrow(0))} \cdot \Theta_\pm$, and hence

$$\bar{H}_x = \frac{\zeta_x}{x_c} \Theta_+ \left(F_\uparrow \cdot e^{-i\sqrt{2}(1-\rho_z)\varphi_\uparrow(0) + i\sqrt{2}\rho_z\varphi_\downarrow(0)} + F_\downarrow \cdot e^{i\sqrt{2}\rho_z\varphi_\uparrow(0) - i\sqrt{2}(1-\rho_z)\varphi_\downarrow(0)} \right) + h.c. \tag{B46}$$

In Eq. (B45), the term $-\frac{4\rho_z^2}{x_c}\Lambda_z^2 = -\frac{4\rho_z^2}{x_c}\mathbb{P}_D$ implies that, the total energy of the doublet coupled to a phase shifted bath will be lowered due to the coupling ρ_z . We hence dub $\frac{\varepsilon_D}{x_c} = J - \frac{4\rho_z^2}{x_c}$ as the effective parameter that enters RG, where ε_D is chosen as dimensionless for convenience. Since we are interested in the phase transition to the LS regime, we will assume $\varepsilon_D > 0$.

The RG flow of Eqs. (B45) and (B46) will be analyzed in Sec. F.

5. Quasiparticle operators and spectral functions in Kondo-type models

We are interested in the spectral function of the physical f -electrons in the original Anderson model, defined by

$$A_f(\omega) = -\frac{1}{\pi} \text{Im} G_f(\omega + i0^+) \tag{B47}$$

where $G_f(\omega)$ can be obtained by analytical continuing the imaginary-time Green's function,

$$G_f(\tau) = -\left\langle T_\tau f_{ls}(\tau) f_{ls}^\dagger(0) \right\rangle \quad G_f(i\omega) = \int_{-\infty}^{\infty} d\tau G_f(\tau) e^{i\omega\tau} \quad (\text{B48})$$

Operators here are in the Heisenberg representation, $f_{ls}(\tau) = e^{H\tau} f_{ls} e^{-H\tau}$. However, to calculate $A_f(\omega)$ in the Kondo or PK models is not so obvious, as the f electron has gone through several SW transformations. After a SW transformation e^{iS} to the low-energy subspace $\mathbb{P}^{(L)}$, it leaves a component of $\tilde{f}_{ls} = \mathbb{P}^{(L)} e^{iS} f_{ls} e^{-iS} \mathbb{P}^{(L)}$. Crucially, in the original Anderson model, the relation $f_{ls} \propto [H - H_0, \psi_{ls}(0)]$ holds as an identity, where H_0 is the Hamiltonian of the bath electrons. Now we show that, to the leading order of $(\frac{1}{U})$, $\tilde{f}_{ls}$ in the low-energy models can be calculated as $\tilde{f}_{ls} \propto [H^{(L)} - H_0^{(L)}, \psi_{ls}(0)]$, where $H^{(L)} = \mathbb{P}^{(L)} e^{iS} H e^{-iS} \mathbb{P}^{(L)}$ and $H_0^{(L)} = \mathbb{P}^{(L)} e^{iS} H_0 e^{-iS} \mathbb{P}^{(L)}$ are the low-energy effective Hamiltonians.

By the above definition,

$$\begin{aligned} \tilde{f}_{ls} &\propto \mathbb{P}^{(L)} e^{iS} [H - H_0, \psi_{ls}(0)] e^{-iS} \mathbb{P}^{(L)} = \mathbb{P}^{(L)} [\tilde{H} - \tilde{H}_0, \tilde{\psi}_{ls}(0)] \mathbb{P}^{(L)} \\ &= \left(\mathbb{P}^{(L)} \tilde{H} \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)} - \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) \tilde{H} \mathbb{P}^{(L)} \right) - \left(\mathbb{P}^{(L)} \tilde{H}_0 \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)} - \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) \tilde{H}_0 \mathbb{P}^{(L)} \right) \end{aligned} \quad (\text{B49})$$

where we have denoted $\tilde{H} = e^{iS} H e^{-iS}$, $\tilde{H}_0 = e^{iS} H_0 e^{-iS}$, and $\tilde{\psi}_{ls}(0) = e^{iS} \psi_{ls}(0) e^{-iS}$ for brevity, and expanded the commutators explicitly. To proceed, we note that $\mathbb{P}^{(L)} \tilde{H} (1 - \mathbb{P}^{(L)}) = 0$ by the construction of the SW transformation (see Sec. B 2), while $\mathbb{P}^{(L)} \tilde{H}_0 (1 - \mathbb{P}^{(L)}) \neq 0$, hence

$$\begin{aligned} \tilde{f}_{ls} &\propto \left(\mathbb{P}^{(L)} \tilde{H} \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)} - \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)} \tilde{H} \mathbb{P}^{(L)} \right) - \left(\mathbb{P}^{(L)} \tilde{H}_0 \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)} - \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)} \tilde{H}_0 \mathbb{P}^{(L)} \right) \\ &\quad - \left(\mathbb{P}^{(L)} \tilde{H}_0 (1 - \mathbb{P}^{(L)}) \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)} - \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) (1 - \mathbb{P}^{(L)}) \tilde{H}_0 \mathbb{P}^{(L)} \right) \\ &= [H^{(L)} - H_0^{(L)}, \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)}] - \left(\mathbb{P}^{(L)} \tilde{H}_0 (1 - \mathbb{P}^{(L)}) \tilde{\psi}_{ls}(0) \mathbb{P}^{(L)} - \mathbb{P}^{(L)} \tilde{\psi}_{ls}(0) (1 - \mathbb{P}^{(L)}) \tilde{H}_0 \mathbb{P}^{(L)} \right) \end{aligned} \quad (\text{B50})$$

In the first term, $\mathbb{P}^{(L)} \tilde{\psi}_{ls} \mathbb{P}^{(L)} = \psi_{ls} + \mathcal{O}(\frac{1}{U^2})$, and the second term itself is of $\mathcal{O}(\frac{1}{U^2})$, as both $\mathbb{P}^{(L)} \tilde{H}_0 (1 - \mathbb{P}^{(L)})$ and $\mathbb{P}^{(L)} \psi (1 - \mathbb{P}^{(L)})$ are of order $\mathcal{O}(\frac{1}{U})$. Therefore, there is

$$\tilde{f}_{ls} \propto [H^{(L)} - H_0^{(L)}, \psi_{ls}(0)] \quad (\text{B51})$$

which by itself is of order $\mathcal{O}(\frac{1}{U})$.

The above result can be understood from another perspective. In the original Anderson model, from the viewpoint of a bath ψ -electron (or in the tunneling experiments, an electron on the tip), an f -electron is nothing but the intermediate process when ψ is scattered at the origin $x = 0$, hence $G_f(\omega)$ is proportional to the scattering $T(\omega)$ -matrix of ψ electrons. After the SW transformation, as the bath electrons remain largely unchanged, namely, $e^{iS} \psi e^{-iS} = \psi + \mathcal{O}(\frac{1}{U})$, one can still extract $G_f(\omega)$ by computing the $T(\omega)$ -matrix in these low-energy effective models. The scattering $T(\omega)$ -matrix will turn out to be given by the Green's function of the operator $\tilde{f}_{ls} = [H^{(L)} - H_0^{(L)}, \psi_{ls}(0)]$ [112–114].

6. Relation to MATBG

In MATBG, each AA-stacking site behaves as a four-orbital (eight-flavor) quantum impurity [47], with the electron operator dubbed as $f_{\beta\eta s}^\dagger$. $s = \uparrow, \downarrow$ denotes the spin, $\eta = \pm$ denotes the graphene valley, and $\beta = 1, 2$ distinguishes the orbital angular momentum (OAM) in each valley as $(-1)^{\beta-1} \eta \bmod 3$. Let us dub the Pauli matrices associated with β, η, s as σ, τ, ς , respectively. The symmetry group consists of charge $U(1)_c$ (generated by $\sigma^0 \tau^0 \varsigma^0$), spin $SU(2)_s$ (generated by $\sigma^0 \tau^0 \varsigma^{x,y,z}$), and valley $U(1)_v$ (generated by $\sigma^0 \tau^z \varsigma^0$). At each f site, per valley, there is a point group D_3 (generated by $C_{3z} = e^{i\frac{2\pi}{3} \sigma^z \tau^z \varsigma^0}$ and $C_{2x} = \sigma^x \tau^0 \varsigma^0$), and the two valleys are linked by $C_{2z} = \sigma^x \tau^x \varsigma^0$. Finally, there is the Kramer's time-reversal $\mathcal{T} = i\sigma^0 \tau^x \varsigma^y K$, where K is complex conjugation. It can be combined with a spin $SU(2)$ rotation $e^{-i\frac{\pi}{2} \sigma^0 \tau^0 \varsigma^y} = -i\sigma^0 \tau^0 \varsigma^y$ to produce the spinless time-reversal symmetry $T = \sigma^0 \tau^x \varsigma^0 K$. We also have $C_{2z} T = \sigma^x \tau^0 \varsigma^0 K$, and $C_{2y} T = \sigma^0 \tau^0 \varsigma^0 K$.

Due to the highly localized nature of the Wannier functions, it is a good approximation that the C_{3z} rotation symmetry (per valley) at the f site can be upgraded to a continuous rotation symmetry [47, 48], so that $\sigma^z \tau^z \varsigma^0$ becomes the generator of the corresponding OAM $U(1)$ charge. Such an upgrade also naturally occurs in the effective impurity problem during the DMFT calculations, where the hybridization function of the f impurity is realized by an auxiliary bath, with the OAM turning into an internal degree of freedom (e.g. see Sec. B 1). In that case, any bilinear or quartic Hamiltonian that conserves OAM mod 3 can

only change OAM by 0, but not 3, 6, etc. Therefore, OAM will be automatically conserved as a continuous rotation symmetry. In this work, we will also adopt this approximation, and treat OAM as a U(1) charge.

It is shown in Ref. [83] that, the microscopic interactions due to vibrating phonons and the atomic-scale Coulomb repulsion (e.g. carbon-atom Hubbard), when projected to an f impurity, can lead to multiplet splittings with the form of

$$H = -\frac{1}{2} \sum_{\beta_1\beta_2\beta'_1\beta'_2} \sum_{\eta s s'} \left[f_{\beta_1\eta s}^\dagger f_{\beta'_1\eta s'}^\dagger \begin{pmatrix} J_a & 0 & 0 & 0 \\ 0 & -J_a & J_b & 0 \\ 0 & J_b & -J_a & 0 \\ 0 & 0 & 0 & J_a \end{pmatrix}_{\beta'_1\beta_1, \beta'_2\beta_2} f_{\beta'_2\eta s'} f_{\beta_2\eta s} \right. \\ \left. + f_{\beta_1\eta s}^\dagger f_{\beta'_1\eta s'}^\dagger \begin{pmatrix} J_a & 0 & 0 & J_b \\ 0 & -J_a & 0 & 0 \\ 0 & 0 & -J_a & 0 \\ J_b & 0 & 0 & J_a \end{pmatrix}_{\beta'_1\beta_1, \beta'_2\beta_2} f_{\beta'_2\eta s'} f_{\beta_2\eta s} + f_{\beta_1\eta s}^\dagger f_{\beta'_1\eta s'}^\dagger \begin{pmatrix} J_e & 0 & 0 & J_d \\ 0 & 0 & J_d & 0 \\ 0 & J_d & 0 & 0 \\ J_d & 0 & 0 & J_e \end{pmatrix}_{\beta'_1\beta_1, \beta'_2\beta_2} f_{\beta'_2\eta s'} f_{\beta_2\eta s} \right] \quad (\text{B52})$$

where the index $(\beta') = (11), (12), (21), (22)$. For the phonon-mediated interactions, $J_{a,b,d,e} > 0$, implying an anti-Hund's nature, while for the carbon-atom Hubbard, $J_{a,b,d,e} < 0$, implying a Hund's nature.

In experimental samples, the degeneracy between the two OAM can be externally broken by heterostrain, and the degeneracy between the two valleys can be spontaneously broken. With electron-doping or hole-doping on such a symmetry-breaking background, the remaining active flavors will form a two-orbital quantum impurity problem, which is nothing but the model introduced in Sec. B 1. We refer to it as the “two-valley” model, where the valley may represent either the original valley or the OAM degree of freedom, as clarified below. We now show how heterostrain or valley order downfolds the original eight-flavor problem to the four-flavor one.

Heterostrain—Heterostrain of various strengths is inevitable in experiments. It explicitly breaks C_{3z} , and leads to a Zeeman splitting on the f site as [61],

$$m_x \cdot [\sigma^x \tau^0 \zeta^0 \cos \varphi_0 + \sigma^y \tau^z \zeta^0 \sin \varphi_0] \quad (\text{B53})$$

Here, φ_0 denotes the azimuthal angle of the heterostrain axis. For a typical heterostrain $\sim 0.2\%$ in experiments, $m_x \approx 10\text{meV}$. The active flavors are the eigen-states of Eq. (B53), which can be parameterized as

$$f_{ls} = \frac{1}{\sqrt{2}} \left(e^{\frac{i}{2}\eta\vartheta_0} f_{1\eta s} + e^{-\frac{i}{2}\eta\vartheta_0} f_{2\eta s} \right) \quad \text{where } l = \eta \quad (\text{B54})$$

where $\vartheta_0 = \varphi_0$ or $\varphi_0 + \pi$ for electron or hole doping, respectively, but the two cases do not need to be distinguished for our purpose. To make connection with Sec. B 1, as the $U(1)_c$ and $SU(2)_s$ symmetries are obvious, we simply check the origin of the $D_\infty = U(1)_v \times Z_2$ symmetry and the C_2T symmetry. Here, $U(1)_v$ is given by the unbroken valley $U(1)$, and the Z_2 factor is generated by C_{2z} that anti-commutes with the valley $U(1)$ generator. For the gauge choice of Eq. (B54), $C_{2z} f_{ls} C_{2z} = f_{\bar{l}s}$. Finally, $C_{2z}T$ acts as $(C_{2z}T) f_{ls} (C_{2z}T)^{-1} = f_{ls}$, which hence serves as the C_2T symmetry discussed in Sec. B 1.

Next, we project the full multiplet splitting in MATBG Eq. (B52) to the active flavors. According to Eq. (B54), such a projection amounts to replacing $f_{1\eta s} \rightarrow \frac{e^{-\frac{i}{2}\eta\vartheta_0}}{\sqrt{2}} f_{ls}$ and $f_{2\eta s} \rightarrow \frac{e^{\frac{i}{2}\eta\vartheta_0}}{\sqrt{2}} f_{ls}$, where $l = \eta$. A crucial observation that simplifies the calculation is that, these complex phases $e^{\pm\frac{i}{2}\eta\vartheta_0}$ are proportional to the OAM of the f operator that they are replacing, while for all non-vanishing matrix elements in Eq. (B52), the OAM adds to 0. Therefore, all complex phases multiply to 1. The final result reads,

$$H = -\frac{1}{2} \sum_{l_1 l'_1 l_2 l'_2} \sum_{s s'} f_{l_1 s}^\dagger f_{l'_1 s'}^\dagger \begin{pmatrix} \frac{J_b}{2} & & & \\ & \frac{J_b}{2} & J_d + \frac{J_e}{2} & \\ & J_d + \frac{J_e}{2} & \frac{J_b}{2} & \\ & & & \frac{J_b}{2} \end{pmatrix}_{l'_1 l_1, l'_2 l_2} f_{l'_2 s'} f_{l_2 s} \quad (\text{B55})$$

Note that the identity component of the above matrix simply contributes to the Hubbard U and does not affect $J_{S,D}$. By comparing with Eq. (B6), one concludes that $J_D = \frac{J_S}{2} = J_d + \frac{J_e}{2}$, as summarized in Table V.

Spontaneous valley orders—A variety of valley orders have been proposed in MATBG, including the valley-polarized order (VP), the Kramer's inter-valley coherent order (KIVC), the spinless- T symmetric inter-valley coherent order (TIVC), and the incommensurate Kekulé spiral order (IKS). Their corresponding order parameters are given below as

$$\sigma^0 \tau^z \zeta^0 \quad \sigma^y (\tau^x \cos \varphi_0 + \tau^y \sin \varphi_0) \zeta^0 \quad \sigma^x (\tau^x \cos \varphi_0 + \tau^y \sin \varphi_0) \zeta^0 \quad \sigma^x (\tau^x \cos(\mathbf{q} \cdot \mathbf{R}) + \tau^y \sin(\mathbf{q} \cdot \mathbf{R})) \zeta^0 \quad (\text{B56})$$

Order	Definition of f_{ls} for $l = \pm$	J_S	J_D	Origin of $D_\infty = U(1)_v \rtimes Z_2$		Origin of C_2T
				$U(1)_v$	Z_2	
Strain	$f_{+s} = \frac{1}{\sqrt{2}} \left(e^{i\frac{\vartheta_0}{2}} f_{1+s} + e^{-i\frac{\vartheta_0}{2}} f_{2+s} \right)$ $f_{-s} = \frac{1}{\sqrt{2}} \left(e^{-i\frac{\vartheta_0}{2}} f_{1-s} + e^{i\frac{\vartheta_0}{2}} f_{2-s} \right)$	$2J_d + J_e$	$J_d + \frac{J_e}{2}$	Valley $U(1)$	C_{2z}	$C_{2z}T$
VP	$f_{+s} = f_{1\eta s}$ $f_{-s} = f_{2\eta s}$	$2J_b$	$2J_a + J_b$	OAM $U(1)$	C_{2x}	$C_{2y}T$
KIVC	$f_{+s} = \frac{1}{\sqrt{2}} \left(e^{i\frac{\vartheta_0}{2}} f_{1+s} - i \cdot e^{-i\frac{\vartheta_0}{2}} f_{2-s} \right)$ $f_{-s} = \frac{1}{\sqrt{2}} \left(e^{i\frac{\vartheta_0}{2}} f_{2+s} + i \cdot e^{-i\frac{\vartheta_0}{2}} f_{1-s} \right)$	J_e	$J_d + \frac{J_e}{2}$	OAM $U(1)$	$C_{2x} \cdot e^{i\pi \frac{\tau^0 - \tau^z}{2}}$	$C_{2y}T \cdot e^{i\vartheta_0 \tau^z} \cdot e^{i\pi \frac{\tau^0 - \tau^z}{2}}$
TIVC (IKS)	$f_{+s} = \frac{1}{\sqrt{2}} \left(e^{i\frac{\vartheta_0}{2}} f_{1+s} + e^{-i\frac{\vartheta_0}{2}} f_{2-s} \right)$ $f_{-s} = \frac{1}{\sqrt{2}} \left(e^{i\frac{\vartheta_0}{2}} f_{2+s} + e^{-i\frac{\vartheta_0}{2}} f_{1-s} \right)$	$2J_b + J_e$	$J_b + \frac{J_e}{2}$	OAM $U(1)$	C_{2x}	$C_{2y}T \cdot e^{i\vartheta_0 \sigma^0 \tau^z \zeta^0}$

TABLE V. Downfolding the four-orbital (eight-flavor) quantum impurity in MATBG to the two-valley (four-flavor) one.

respectively. φ_0 characterizes the IVC angles, while in IKS, such IVC angle is “spiraling” across different moiré unit cells $\mathbf{R}$ with some wave-vector $\mathbf{q}$. Viewed locally from one f impurity, IKS is barely distinguishable from TIVC, hence we treat them identically below. In this work, we do not intend to discuss which order is more likely to appear in MATBG; instead, we only discuss that if any of the above order forms, what two-valley impurity problem they will give rise to.

The active flavors are also given by eigenstates of the order parameters Eq. (B56), which we tabulate in Table V. As valley degeneracy is broken, l among the active flavors labels OAM, and hence the effective $U(1)_v$ symmetry in the two-valley model corresponds to the OAM $U(1)$ symmetry in the original model. For VP and TIVC (IKS), the degeneracy of opposite OAM is protected by a Z_2 group generated by C_{2x} , which will combine with $U(1)_v$ to span the D_∞ valley group. For KIVC, it is protected by C_{2x} dressed by a valley $U(1)$ rotation, $C_2 = C_{2x} \cdot e^{i\pi \frac{\tau^z - \tau^0}{2}}$, although both C_{2x} and valley $U(1)$ are individually broken. This new action shares the same algebra as C_{2x} : $C_2^2 = 1$, and C_2 anti-commutes with the $U(1)_v$ generator $\sigma^z \tau^z \zeta^0$. Consequently, KIVC also enjoys the D_∞ valley group. As for the time-reversal C_2T , it is fulfilled by $C_{2y}T$, or $C_{2y}T$ dressed by some valley $U(1)$ rotations. One can directly verify that for the wave-functions tabulated in Table V, and the corresponding definition of C_2 and C_2T actions, there are $C_2 f_{ls} C_2^{-1} = f_{\bar{l}s}$, and $(C_2T) f_{ls} (C_2T)^{-1} = f_{ls}$.

Finally, we also project the multiplet splitting interaction Eq. (B52) to the active flavors. For VP, such projection is very straightforward, by simply keeping the first line of Eq. (B52). For KIVC, we replace $f_{\beta\eta s} \rightarrow \frac{e^{-\frac{1}{2}\eta\vartheta_0}}{\sqrt{2}} e^{i\frac{\pi}{2}l\frac{1-\eta}{2}} f_{ls}$ where $l = \beta\eta \bmod 3$. Calculation shows that

$$H = -\frac{1}{2} \sum_{l_1 l'_1 l_2 l'_2} \sum_{ss'} f_{l_1 s}^\dagger f_{l'_1 s'}^\dagger \begin{pmatrix} \frac{J_d}{2} & & \\ & -\frac{J_d}{2} & \frac{J_e}{2} \\ & \frac{J_e}{2} & -\frac{J_d}{2} \\ & & & \frac{J_d}{2} \end{pmatrix} f_{l'_2 s'} f_{l_2 s} \quad (B57)$$

By comparison with Eq. (B6), we find $J_S = J_e$, and $J_D - \frac{J_S}{2} = J_d$ hence $J_D = J_d + \frac{J_e}{2}$. For TIVC, we replace $f_{\beta\eta s} \rightarrow \frac{e^{+i\eta\frac{\vartheta_0}{2}}}{\sqrt{2}} f_{ls}$, where $l = \beta\eta \bmod 3$. Calculation shows that

$$H = -\frac{1}{2} \sum_{l_1 l'_1 l_2 l'_2} \sum_{ss'} f_{l_1 s}^\dagger f_{l'_1 s'}^\dagger \begin{pmatrix} \frac{J_d}{2} & & \\ & \frac{J_d}{2} & J_b + \frac{J_e}{2} \\ & J_b + \frac{J_e}{2} & \frac{J_d}{2} \\ & & & \frac{J_d}{2} \end{pmatrix} f_{l'_2 s'} f_{l_2 s} \quad (B58)$$

By comparison with Eq. (B6), we read off $J_D = \frac{J_S}{2} = J_b + \frac{J_e}{2}$.

This subsection demonstrates that projecting onto different active orbitals yields the same two-valley model. In addition to the $J_{S,D}$ values obtained from the projection (Table V), several other effects may affect the competition between S , D , T states. For example, as discussed at the end of Sec. B4, the ρ_z coupling further lowers the energy of D states. Other factors include fluctuations involving the inactive orbitals and the deviations of the actual active Wannier functions from the simply projected ones. But these factors will not change the form of the two-valley Hamiltonian, which is restricted by symmetry. Therefore, in this work we will not take the values of $J_{S,D}$ in Table V but treat them as free parameters.

C. Exact solution to the pair-Kondo model at $\lambda_x = 0$

1. Finite-size spectrum

When $\lambda_x = 0$, $\Lambda_z = \pm 1$ is a good quantum number of the system, and the Hamiltonian $\bar{H}_{\text{PK}}$ (Eq. (B39)) is diagonal in the quantum numbers $n_\chi(q) = b_\chi^\dagger(q)b_\chi(q)$, N_χ , Λ_z . Thus, one can simply enumerate these quantum numbers and read the eigenenergy.

A simpler method uses the original fermion representation of $\bar{H}_{\text{PK}}$ (Eq. (B26)). According to the discussion discussed around Eq. (A33), for a given Λ_z , λ_z will introduce a phase shift $l\Lambda_z\rho_z$ for the fermion mode $\psi_{ls}(x)$. Therefore, the energy spectrum in a Λ_z sector is generated by the free-fermion Hamiltonian

$$H = \sum_{ls} \sum_{k \in \mathcal{Q}_l[\Lambda_z]} k : d_{ls}^\dagger(k) d_{ls}(k) : \quad (\text{C1})$$

where

$$\mathcal{Q}_l[\Lambda_z] = \frac{2\pi}{L} \left(\mathbb{Z} - \frac{P_{\text{bc}}}{2} + l \cdot \Lambda_z \cdot \rho_z \right). \quad (\text{C2})$$

Following the convention in Sec. A1, the vacuum state $|0\rangle_0$ respected by the normal ordering occupies all *negative and zero* levels.

If $P_{\text{bc}} = 0$, when $\rho_z = 0$, all the $N_{ls} = 0$ or -1 states (in both $\Lambda_z = \pm$ sectors) are degenerate, leading to a $2^4 \times 2$ -fold degeneracy. With an infinitesimal $\rho_z > 0$ ($\rho_z < 0$), in *each* $\Lambda_z = \pm 1$ subspace, the $N_{l=\Lambda_z,s} = -1$ (0), $N_{l=-\Lambda_z,s} = 0$ (-1) state becomes the only ground state. If $P_{\text{bc}} = 1$, the ground state degeneracy is always two, and ρ_z , whose limits are $\pm \frac{1}{2}$, cannot lead to a level crossing.

2. Impurity susceptibility

When only correlation functions are of concern, we can omit the $\mathcal{O}(L^{-1})$ terms in Eq. (B39) and obtain a free-boson Hamiltonian

$$\bar{H}_0 = \sum_\chi \int \frac{dx}{4\pi} : (\partial_x \phi_\chi(x))^2 : = \sum_\chi \sum_{q>0} q b_\chi^\dagger(q) b_\chi(q). \quad (\text{C3})$$

The partition function is given by $Z_0 = \text{Tr}[e^{-\beta \bar{H}_0}] = \text{Tr}[e^{-\beta \bar{H}_0}]$, where $\bar{H}_0 = U H_0 U^\dagger$ and $\beta = 1/T$ is the inverse temperature. The average over some operator $\bar{X}$ (written in the original gauge) reads

$$\langle X \rangle_0 = \frac{1}{Z_0} \text{Tr} [X \cdot e^{-\beta(H_0 + H_z)}] = \langle \bar{X} \rangle_{\bar{0}} = \frac{1}{Z_0} \text{Tr} [\bar{X} \cdot e^{-\beta \bar{H}_0}], \quad (\text{C4})$$

where $\bar{X} = U X U^\dagger$, $U = e^{2i\rho_z \Lambda_z \phi_v(0)}$. The subscripts 0 and $\bar{0}$ represent average with respect to H_0 and $\bar{H}_0$, respectively. At zero temperature, the expectation value becomes

$$\langle \bar{X} \rangle_{\bar{0}} = \frac{1}{2} \sum_{\Lambda_z = \pm} \langle \Lambda_z; \bar{G} | \bar{X} | \Lambda_z; \bar{G} \rangle, \quad (\text{C5})$$

where $|\Lambda_z; \bar{G}\rangle = |\Lambda_z\rangle \otimes |\bar{G}\rangle$ and $|\bar{G}\rangle$ is the free boson vacuum independent of Λ_z .

Since Λ_z is conserved, $\Lambda_z(\tau) = e^{\tau H} \Lambda_z e^{-\tau H} = \Lambda_z$, the longitudinal correlation function

$$\chi_z(\tau) = -\langle T_\tau \Lambda_z(\tau) \Lambda_z(0) \rangle_0 = -1 \quad (\text{C6})$$

does not decay at any temperature, leading to a Curie's law of the static susceptibility, i.e., $\chi_z \sim \frac{1}{T}$.

Next we compute the transverse correlation function, $\chi_x(\tau) = -\langle T_\tau \Lambda_-(\tau) \Lambda_+(0) \rangle_0 = -\langle T_\tau \bar{\Lambda}_-(\tau) \bar{\Lambda}_+(0) \rangle_{\bar{0}}$. Here

$$\bar{\Lambda}_\pm(\tau) = U e^{\tau H_0} \Lambda_\pm e^{-\tau H_0} U^\dagger = e^{\tau \bar{H}_0} (\Lambda_\pm e^{\pm 4i\rho_z \phi_v(0)}) e^{-\tau \bar{H}_0} = \Lambda_\pm e^{\pm 4i\rho_z \phi_v(\tau,0)}. \quad (\text{C7})$$

We have used Eq. (B38) in the second step. $\phi_v(\tau, x) = e^{\tau \bar{H}_0} \phi_v(x) e^{-\tau \bar{H}_0}$ denotes the free evolution of the boson field. Therefore,

$$\chi_x(\tau) = -\left\langle T_\tau \Lambda_- e^{-4i\rho_z \phi_v(\tau,0)} \Lambda_+ e^{4i\rho_z \phi_v(0,0)} \right\rangle_{\bar{0}} = -\left\langle \Lambda_- \Lambda_+ \right\rangle_{\bar{0}} \left\langle T_\tau e^{-4i\rho_z \phi_v(\tau,0)} e^{4i\rho_z \phi_v(0,0)} \right\rangle_{\bar{0}} \quad (\text{C8})$$

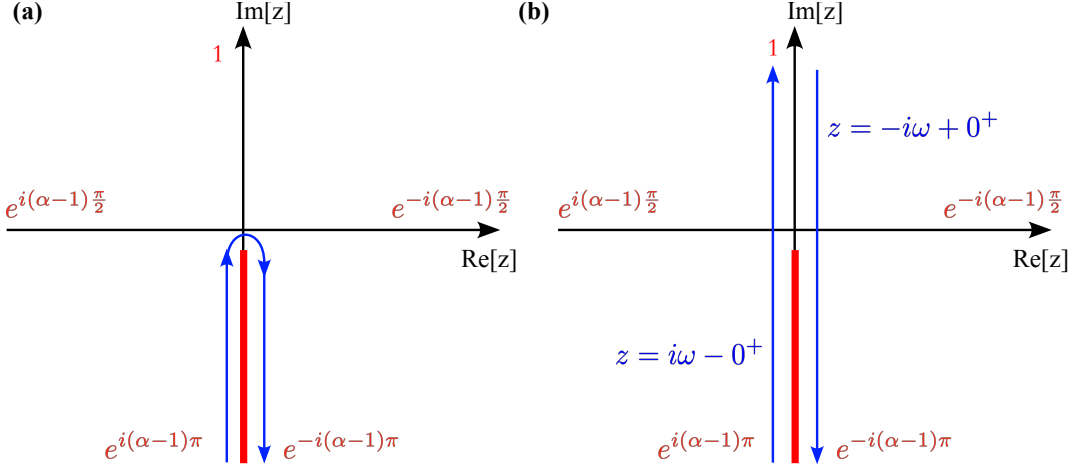


FIG. 6. Contour integral about $f(z) = (-iz + 0^+)^{\alpha-1}$. The bold red line represents the branch-cut of $f(z)$. The red numbers 1, $e^{\pm(\alpha-1)\frac{\pi}{2}}$, $e^{\pm(\alpha-1)\pi}$ represent $f(z)/|f(z)|$ in at $z = iy, \mp x, \mp 0^+ - iy$, respectively, where $x, y > 0$.

This step exploited the fact that the eigenstates are direct products of impurity and bath fields. $\langle \Lambda_- \Lambda_+ \rangle_0 = \frac{1}{2}$ by definition, and the bath correlation functions can be looked up in Eq. (A59). Similar expressions can be derived for the retarded Green's function. We summarize that

$$\chi_x(\tau) = -\langle T_\tau \Lambda_-(\tau) \Lambda_+(0) \rangle_0 = -\frac{1}{2} \left(\frac{\pi T x_c}{\sin[\pi T|\tau| + \pi T x_c]} \right)^{16\rho_z^2} T \xrightarrow{0^+} -\frac{1}{2} \left(\frac{x_c}{|\tau| + x_c} \right)^{16\rho_z^2} \quad (C9)$$

$$C_x^R(t) = -i\theta(t) \langle [\Lambda_-(t), \Lambda_+(0)] \rangle_0 \xrightarrow{T \rightarrow 0^+} -\theta(t) \frac{i}{2} \left[\left(\frac{x_c}{it + x_c} \right)^{16\rho_z^2} - \left(\frac{x_c}{-it + x_c} \right)^{16\rho_z^2} \right] \quad (C10)$$

In particular, for $\rho_z < \rho_z^* = \frac{1}{4}$, where ρ_z^* is another solvable fixed point, the power $\alpha = 16\rho_z^2 < 1$.

The transverse susceptibility in the real-frequency domain is defined as $\chi_x^R(\omega) = \int_{-\infty}^{\infty} dt \chi_x^R(t) e^{i\omega t}$. In numerical calculations such as Numerical Renormalization Group, $\text{Im}[\chi_x^R(\omega)]$ can be computed using the Lehmann spectral representation, where only eigenstates with the energy ω contribute. Thus, $\text{Im}[\chi_x^R(\omega)]$ is important to characterize the low-energy physics. Here we first construct a Mastubara $\chi_x(i\omega)$ that reproduces $\chi_x(\tau) = -\frac{1}{2} \left| \frac{x_c}{\tau} \right|^\alpha$ for $|\tau| \gg x_c$, and then derive $\chi_x^R(\omega)$ by analytical continuation. We do not concern ourselves with short-time behaviors at $\tau \sim x_c$. Consider the integral

$$I(\tau) = \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\tau} (-i\omega + \varepsilon)^{\alpha-1}. \quad (C11)$$

We introduce the function

$$f(z) = (-iz + \varepsilon)^{\alpha-1} \quad (C12)$$

and choose it to be analytical in the upper complex z -plane ($\text{Im}[z] \geq 0$). As shown in Fig. 6, $f(z)$ has a branch-cut at $z = -iy$ ($y \geq \varepsilon$). When $\tau < 0$, we change the integral in $I(\tau)$ to a contour integral enclosing the upper z -plane. Since $f(z)$ is analytical there, $I(\tau) = 0$ for $\tau < 0$. When $\tau > 0$, we change integral to a contour integral enclosing the lower z -plane, where a branch-cut lies. We deform the contour to approach the branch-cut, as illustrated by the blue line in Fig. 6(a). Then we have

$$I(\tau) = -\frac{i}{2\pi} \theta(\tau) \int_{\varepsilon}^{\infty} dy e^{-y\tau} (f(\varepsilon - iy) - f(-\varepsilon - iy)) + \mathcal{O}(\varepsilon f(\varepsilon)) \quad (C13)$$

where $\mathcal{O}(\varepsilon f(\varepsilon)) = \mathcal{O}(\varepsilon^\alpha)$ vanishes in the $\varepsilon \rightarrow 0^+$ limit as long as $\alpha > 0$. According to the definition of the branch of $f(\omega)$, we have $f(\pm\varepsilon - iy)/f(\pm\varepsilon + iy) = e^{\mp i(\alpha-1)\pi}$ for $y \gg \varepsilon$. Thus,

$$I(\tau) = -\frac{i}{2\pi} \theta(\tau) \lim_{\varepsilon \rightarrow 0^+} \int_{\varepsilon}^{\infty} dy e^{-y\tau} ((y - \varepsilon)^2 + \varepsilon^2)^{\frac{\alpha-1}{2}} (e^{-i\pi(\alpha-1)} - e^{i\pi(\alpha-1)}) = \frac{\sin((1-\alpha)\pi)}{\pi} \frac{\theta(\tau)}{|\tau|^\alpha} \Gamma(\alpha) \quad (C14)$$

with $\Gamma(\alpha)$ being the Γ -function. Therefore, the imaginary-time correlation function is reproduced as

$$\chi_x(\tau) = -\frac{1}{2} \cdot \frac{\pi x_c^\alpha}{\sin((1-\alpha)\pi) \cdot \Gamma(\alpha)} \cdot (I(\tau) + I(-\tau)) . \quad (\text{C15})$$

Correspondingly, the Matsubara Green's function is

$$\chi_x(i\omega) = -\frac{1}{2} \cdot \frac{\pi x_c^\alpha}{\sin((1-\alpha)\pi) \cdot \Gamma(\alpha)} \left((-i\omega + 0^+)^{\alpha-1} + (i\omega + 0^+)^{\alpha-1} \right) . \quad (\text{C16})$$

$\chi_x(i\omega)$ is real and even in ω , as required by the Lehmann spectral representation of bosonic Matsubara Green's function. The retarded Green's function can be obtained by analytic continuation ($i\omega \rightarrow \omega + i0^+$):

$$\begin{aligned} \chi_x^R(\omega) &= -\frac{1}{2} \cdot \frac{\pi \cdot x_c^\alpha}{\sin((1-\alpha)\pi) \cdot \Gamma(\alpha)} \left((-\omega - i0^+)^{\alpha-1} + (\omega + i0^+)^{\alpha-1} \right) \\ &= -\frac{1}{2} \cdot \frac{\pi \cdot x_c^\alpha}{\sin((1-\alpha)\pi) \cdot \Gamma(\alpha)} \cdot |\omega|^{\alpha-1} \cdot \left(1 + e^{i\pi(1-\alpha)\text{sgn}(\omega)} \right) . \end{aligned} \quad (\text{C17})$$

One should interpret $(-\omega - i0^+)^{\alpha-1}$ and $(\omega + i0^+)^{\alpha-1}$ as $f(z = -i\omega + 0^+)$ and $f(z = i\omega - 0^+)$, respectively (Fig. 6(b)). Its imaginary part is

$$\text{Im}[\chi_x^R(\omega)] = -\frac{x_c^\alpha |\omega|^{\alpha-1} \text{sgn}(\omega)}{2\Gamma(\alpha)} . \quad (\text{C18})$$

It satisfies $\text{Im}[\chi_x^R(\omega > 0)] < 0$ and $\text{Im}[\chi_x^R(\omega)] = -\text{Im}[\chi_x^R(-\omega)]$, as required by the Lehmann spectral representation.

In a practical numerical calculation, high-energy peaks may appear in $\text{Im}[\chi_x^R(\omega)]$, which, through the Kramers-Kronig relation, will lead to a smooth background to $\text{Re}[\chi_x^R(\omega)]$ for low-energy ω . As a result, while the low-energy behavior of $\text{Im}[\chi_x^R(\omega)]$ is universal, that of $\text{Re}[\chi_x^R(\omega)]$ is not.

D. RG analysis of the pair-Kondo model

As we have revealed in Eq. (B39), the impurity only couples to the ϕ_v boson field. Here we omit all the other degrees of freedoms and focus on the simplified effective model

$$\overline{H}_v = \int dx \frac{(\partial_x \phi_v(x))^2}{4\pi} + \frac{\lambda_x}{x_c} \left(\Lambda_+ F_v \cdot e^{-2i(1-2\rho_z)\phi_v(0)} + \Lambda_- F_v^\dagger \cdot e^{2i(1-2\rho_z)\phi_v(0)} \right), \quad (D1)$$

where $\mathcal{O}(L^{-1})$ terms are omitted. The overline indicates that $\overline{H}_v = U H_v U^\dagger$ is transformed from the original representation by $U = e^{2i\rho_z \Lambda_z \phi_v(0)}$. We write the total Hamiltonian as $\overline{H}_v = \overline{H}_{v,0} + \overline{H}_x$, where $\overline{H}_{v,0}$ is the Hamiltonian in the $\lambda_x = 0$ limit, and $\overline{H}_x$ is the λ_x -coupling term. Since $\overline{H}_{v,0}$ is solvable, we will treat $\overline{H}_x$ as a perturbation in this section.

We express the correction to partition function contributed by $\overline{H}_x$ as

$$\delta Z = \frac{Z}{Z_0} = e^{-\beta \cdot \delta F} = \left\langle T_\tau \exp \left(- \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau \overline{H}_x(\tau) \right) \right\rangle_{\overline{0}}. \quad (D2)$$

Here δF is the (additive) correction to the free energy, $\beta = 1/T$ is the inverse temperature, the subscript $\overline{0}$ represents ensemble average with respect to $\overline{H}_{v,0}$, T_τ is the time-ordering operator, and

$$\overline{H}_x(\tau) = e^{\tau \overline{H}_{v,0}} \cdot \overline{H}_x \cdot e^{-\tau \overline{H}_{v,0}} = \frac{\lambda_x}{x_c} \left(\Lambda_+(\tau) F_v(\tau) \cdot e^{-i\gamma \phi_v(\tau,0)} + \Lambda_-(\tau) F_v^\dagger(\tau) \cdot e^{i\gamma \phi_v(\tau,0)} \right) \quad (D3)$$

is the coupling Hamiltonian in the interaction picture. The exponent γ is defined as

$$\gamma = 2(1 - 2\rho_z). \quad (D4)$$

Notice that $\Lambda_\pm(\tau) = \Lambda_\pm$ and $F_v(\tau) = F_v$ because $\overline{H}_{v,0}$ commute with $\Lambda_\pm$ and F_v . However, we still explicitly keep the τ index for the convenience of time ordering.

1. Coulomb gas analog

The partition function in Eq. (D2) can be as a series sum in terms of λ_x :

$$\delta Z = 1 + \delta Z_2 + \delta Z_4 + \dots \quad (D5)$$

where the $2n$ -th order correction is

$$\delta Z_{2n} = \frac{1}{(2n)!} \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau_{2n} \dots \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau_1 \langle T_\tau \overline{H}_x(\tau_{2n}) \dots \overline{H}_x(\tau_1) \rangle_{\overline{0}} = \int_{(-\frac{\beta}{2}, \frac{\beta}{2})}^{>0} d^{2n} \tau \langle \overline{H}_x(\tau_{2n}) \dots \overline{H}_x(\tau_1) \rangle_{\overline{0}} \quad (D6)$$

For the average over $\overline{0}$ to be non-vanishing, the operator string $\overline{H}_x(\tau_{2n}) \dots \overline{H}_x(\tau_1)$ cannot accumulate the Λ_z or N_v charges, which are preserved by $\overline{H}_v$. Thus, odd-order terms δZ_{2n+1} hence vanish. In the last step, we explicitly chose one of the $(2n)!$ time-ordered integral domains, and introduced an abbreviation for the corresponding integral domain and integral measure,

$$\int_{(-\frac{\beta}{2}, \frac{\beta}{2})}^{>0} d^{2n} \tau = \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau_{2n} \int_{-\frac{\beta}{2}}^{\tau_{2n}} d\tau_{2n-1} \dots \int_{-\frac{\beta}{2}}^{\tau_3} d\tau_2 \int_{-\frac{\beta}{2}}^{\tau_2} d\tau_1 \quad (D7)$$

The $\frac{1}{(2n)!}$ factor is canceled by adding up all such domains.

To evaluate the expectation value over an operator $\overline{X}$ that commutes with C_{2x} (such as δZ_{2n}), it suffices to look at the $\Lambda_z = +$ sector of the eigenstates of $\overline{H}_0$, because the other sector produces the same expectation value,

$$\langle \overline{X} \rangle_{\overline{0}} = \langle \overline{X} \rangle_{\overline{0},+}. \quad (D8)$$

We will exploit this property henceforth, but will omit the subscript $\overline{0}, +$ for brevity, unless otherwise mentioned. Also, as in this section we will only encounter ϕ fields located at $x = 0$, we will omit their spatial argument.

At each τ_j in δZ_{2n} , we should pick either the Λ_+ term or the Λ_- term from $\overline{H}_x(\tau_j)$. We now analyze the general structure of the non-vanishing terms in δZ_{2n} :

1. There is a common factor $\left(\frac{\lambda_x}{x_c}\right)^{2n}$.
2. Starting with the $\Lambda_z = +$ state before τ_1 , we can only flip Λ_z down and up alternately. Consequently, we must choose the Λ_- term at all τ_{2k+1} and the Λ_+ term at all τ_{2k} . The staggered string of impurity operators can be factored out, and produces $\langle \Lambda_+ \Lambda_- \cdots \Lambda_+ \Lambda_- \rangle_{\vec{0},+} = 1$.
3. Due to (2), the operator string of vertex operators ($e^{\pm i\gamma\phi_v}$) is also fixed. It gives the factor

$$\left\langle e^{-i\gamma\phi_v(\tau_{2n})} e^{i\gamma\phi_v(\tau_{2n-1})} \cdots e^{-i\gamma\phi_v(\tau_2)} e^{i\gamma\phi_v(\tau_1)} \right\rangle = \exp \left[- \sum_{j>i} (-1)^{j-i} \gamma^2 \ln \left(\frac{\pi T x_c}{\sin(\pi T(\tau_j - \tau_i) + \pi T x_c)} \right) \right], \quad (\text{D9})$$

where Eq. (A61) is exploited. Remarkably, it is equivalent to the partition function of $2n$ classical particles on a line, carrying $\pm\gamma$ charges in a staggered pattern, and interacting through the logarithmic (two-dimensional) Coulomb force. This is known as the Coulomb gas analog [107, 108]. x_c plays the role as a short-distance cutoff in this analog.

4. Due to (2), the Klein factors must compose a string of the form $F_v F_v^\dagger \cdots F_v F_v^\dagger = 1$.
5. Since x_c simply plays the role of a short-distance (high-energy) cutoff, various ways to implement it should agree on the physical output. For convenience, we will use the integral measure

$$\int_{(-\frac{\beta}{2}, \frac{\beta}{2})}^{>x_c} d^{2n}\tau = \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau_{2n} \int_{-\frac{\beta}{2}}^{\tau_{2n}-x_c} d\tau_{2n-1} \cdots \int_{-\frac{\beta}{2}}^{\tau_3-x_c} d\tau_2 \int_{-\frac{\beta}{2}}^{\tau_2-x_c} d\tau_1 \quad (\text{D10})$$

and simultaneously replace all $\frac{\pi T x_c}{\sin(\pi T(\tau_j - \tau_i) + \pi T x_c)}$ with $\frac{\pi T x_c}{\sin(\pi T(\tau_j - \tau_i))}$.

In summary, δZ_{2n} can be written as

$$\delta Z_{2n} = \left(\frac{\lambda_x}{x_c}\right)^{2n} \int_{(-\frac{\beta}{2}, \frac{\beta}{2})}^{>x_c} d^{2n}\tau \cdot \prod_{j>i} \left(\frac{\pi T x_c}{\sin(\pi T(\tau_j - \tau_i))} \right)^{-(-1)^{j-i} \gamma^2} \quad (\text{D11})$$

To gain some insights into the perturbation theory, let us calculate the lowest order correction δZ_2 in the zero-temperature limit ($T \rightarrow 0^+$).

$$\delta Z_2 = \frac{\lambda_x^2}{x_c^2} \int_{-1/(2T)}^{1/(2T)} d\tau_2 \int_{-1/(2T)}^{\tau_1-x_c} d\tau_1 \left(\frac{x_c}{\tau_2 - \tau_1} \right)^{\gamma^2} = \frac{1}{x_c T} \cdot \frac{\lambda_x^2}{\gamma^2 - 1} \left(1 - (2x_c T)^{\gamma^2-1} \right). \quad (\text{D12})$$

Correspondingly, the lowest order correction to the energy $\delta E_2 = -T \cdot \ln \delta Z$ is

$$\delta E_2 = -\frac{1}{x_c} \cdot \frac{\lambda_x^2}{\gamma^2 - 1} \left(1 - (2x_c T)^{\gamma^2-1} \right). \quad (\text{D13})$$

For $\rho_z < \rho_z^* = \frac{1}{4}$, $\gamma > 1$ and $(2x_c T)^{\gamma^2-1}$ vanishes in the $x_c \rightarrow 0^+$, $T \rightarrow 0^+$ limit. However, if $\gamma \leq 1$, the $(2x_c T)^{\gamma^2-1}$ term diverges, suggesting invalidity of the λ_x -expansion. Therefore, $\gamma > 1$ or $\rho_z < \frac{1}{4}$ is necessary to validate the perturbation theory. Further, to justify the perturbation theory, the second-order correction should be smaller than the typical energy scale (x_c^{-1}) of the unperturbed system. Thus, the perturbative regime should be

$$\text{perturbative regime :} \quad \lambda_z < \frac{1}{2}, \quad \lambda_x^2 \lesssim \gamma^2 - 1. \quad (\text{D14})$$

Interestingly, the model at $\rho_z^* = \frac{1}{4}$ can be mapped to a solvable free-fermion system by reformionizing $\frac{F_v}{\sqrt{2\pi x_c}} e^{-i\phi_v}$ to a new fermion operator. This limit is similar to the ‘‘Toulouse line’’ of the single-channel Kondo problem [98, 104] and represents the strong coupling Fermi liquid phase.

2. Flow equations

We will take the order of limits $\lim_{T \rightarrow 0^+} \lim_{x_c \rightarrow 0^+} \lim_{L \rightarrow \infty}$ in the RG analysis in this subsection. We can replace all the $\frac{\pi T x_c}{\sin(\pi T(\tau_j - \tau_i))}$ factors in Eq. (D11) by $\frac{x_c}{\tau_j - \tau_i}$ in this limit.

Rescale all the coordinates as $\tau_i = b\tau'_i$, where $b = e^{d\ell} > 1$, and then relabel τ'_i as τ . The partition function in Eq. (D11) becomes

$$\delta Z_{2n} = \frac{\lambda_x^{2n} \cdot b^{2n-\gamma^2 n}}{x_c^{2n}} \int_{(-\frac{\beta}{2b}, \frac{\beta}{2b})}^{> x_c b^{-1}} d^{2n} \tau \prod_{j>i} \left(\frac{x_c}{\tau_j - \tau_i} \right)^{-(-1)^{j-i} \gamma^2}. \quad (\text{D15})$$

We can absorb the factor $b^{1-\frac{\gamma^2}{2}}$ into λ_x and define it as the renormalized parameter, i.e., $\lambda_x(\ell + d\ell) = \lambda_x(\ell) \cdot e^{d\ell(1-\frac{\gamma^2}{2})}$. The tree-level flow equation for λ_x immediately follows

$$\frac{d\lambda_x}{d\ell} = \left(1 - \frac{\gamma^2}{2} \right) \lambda_x. \quad (\text{D16})$$

One can alternatively obtain this result by a simple power counting. According to the discussion below Eq. (A59), the scaling dimensions of vertex operators $e^{\pm i\gamma\phi_v}$ is $\frac{\gamma^2}{2}$. To ensure the Hamiltonian $\bar{H}_x$ has the correct scaling dimension $[\bar{H}_x] = 1$, the coupling constant must have $[\lambda_x] = 1 - \frac{\gamma^2}{2}$. λ_x is relevant, marginal, and irrelevant for $\gamma < \sqrt{2}$, $\gamma = \sqrt{2}$, and $\gamma > \sqrt{2}$, respectively.

To obtain the flow of γ , we integrate out “high-energy” configurations as virtual processes. The $2n$ -th order partition function has the form $\delta Z_{2n} = \delta Z_{2n,0} + \delta Z_{2n,1} + \mathcal{O}(d\ell^2)$, where all adjacent particles in $\delta Z_{2n,0}$ are separated by a least distance x_c , and one adjacent particle-pair (say τ_{i+1}, τ_i) in $\delta Z_{2n,1}$ have a distance $x_c b^{-1} < \tau_{i+1} - \tau_i < x_c$. Since adjacent particles carry opposite charges, we term the pair (τ_{i+1}, τ_i) as a dipole. Multiple dipole excitations contribute the $\mathcal{O}(d\ell^2)$ term and will be neglected. We integrate out the dipoles and re-organize the low-energy terms into a new partition function, $\delta Z' = \sum_{n=0}^{\infty} \delta Z'_{2n}$, where $\delta Z'_{2n}$ contains $2n$ low-energy particles. We examine the free-energy

$$\begin{aligned} \delta F &= -T \cdot \ln [\delta Z] = -T \cdot \ln \left[1 + \sum_{n=1}^{\infty} \delta Z_{2n,0} + \sum_{n=1}^{\infty} \delta Z_{2n,1} \right] = -T \cdot \ln \left[1 + \delta Z_{2,1} + \sum_{n=1}^{\infty} (\delta Z_{2n,0} + \delta Z_{2n+2,1}) \right] \\ &= -T \cdot \ln (1 + \delta Z_{2,1}) - T \cdot \ln \left[(1 + \delta Z_{2,1})^{-1} \sum_{n=1}^{\infty} (\delta Z_{2n,0} + \delta Z_{2n+2,1}) \right] \\ &= -T \cdot \ln (1 + \delta Z_{2,1}) - T \cdot \ln \left[1 + \sum_{n=1}^{\infty} (\delta Z_{2n,0} + \delta Z_{2n+2,1} - \delta Z_{2n,0} \delta Z_{2,1}) + \mathcal{O}(d\ell^2) \right]. \end{aligned} \quad (\text{D17})$$

Here $-T \cdot \ln(1 + \delta Z_{2,1})$ is the “high-energy” free-energy contributed by the inner degree of freedom of the dipole. The second term is the “low-energy” free-energy, where Coulomb interaction is screened by the dipole. We thus conclude

$$\delta Z'_{2n} = \delta Z_{2n,0} + \delta Z_{2n+2,1} - \delta Z_{2n,0} \delta Z_{2,1} \quad (\text{D18})$$

serves as the effective $2n$ -particle partition function for the low-energy particles.

Let us first compute $\delta Z_{2,1}$,

$$\delta Z_{2,1} = \left(\frac{\lambda_x}{x_c} \right)^2 \cdot b^{2-\gamma^2} \cdot \int_{-\frac{1}{2bT}}^{\frac{1}{2bT}} d\tau_2 \int_{\tau_2 - x_c}^{\tau_2 - x_c b^{-1}} d\tau_1 \left(\frac{x_c}{\tau_2 - \tau_1} \right)^{\gamma^2} = \frac{\lambda_x^2}{x_c T} \cdot d\ell + \mathcal{O}(d\ell^2) \quad (\text{D19})$$

Since the integral range over τ_1 is proportional to $d\ell$, we can safely omit all the $\mathcal{O}(d\ell)$ factors elsewhere.

Next, we compute $\delta Z_{4,1}$ and see how it renormalizes $\delta Z_{2,0}$. The calculation for the renormalization of $\delta Z_{2n,0}$ with generic n parallels with that for $\delta Z_{4,1}$. $\delta Z_{4,1}$ consists of three terms, $\delta Z_{4,1} = \sum_{i=1}^3 \delta Z_{4,1}^{(i+1,i)}$, where $\delta Z_{2n+2,1}^{(i+1,i)}$ has a dipole formed by τ_{i+1} and τ_i . The first term is

$$\begin{aligned} \delta Z_{4,1}^{(2,1)} &= \frac{\lambda_x^4}{x_c^4} \int_{-\frac{1}{2bT}}^{\frac{1}{2bT}} d\tau_4 \int_{-\frac{1}{2bT}}^{\tau_4 - x_c} d\tau_3 \int_{-\frac{1}{2bT}}^{\tau_3 - x_c} d\tau_2 \int_{\tau_2 - x_c}^{\tau_2 - x_c/b} d\tau_1 \exp \left(\gamma^2 \sum_{j>i} (-1)^{j-i} \ln \left(\frac{\tau_j - \tau_i}{x_c} \right) \right) \\ &= \frac{\lambda_x^2}{x_c^2} \cdot \frac{\lambda_x^2 d\ell}{x_c} \int_{-\frac{1}{2bT}}^{\frac{1}{2bT}} d\tau_4 \int_{-\frac{1}{2bT}}^{\tau_4 - x_c} d\tau_3 \int_{-\frac{1}{2bT}}^{\tau_3 - x_c} d\tau_2 \exp \left(-\gamma^2 \ln \left(\frac{\tau_4 - \tau_3}{x_c} \right) + \gamma^2 \ln \left(\frac{\tau_4 - \tau_2}{\tau_4 - \tau_2 + x_c} \right) + \gamma^2 \ln \left(\frac{\tau_3 - \tau_2 + x_c}{\tau_3 - \tau_2} \right) \right) \\ &= \frac{\lambda_x^2}{x_c^2} \cdot \frac{\lambda_x^2 d\ell}{x_c} \int_{-\frac{1}{2bT}}^{\frac{1}{2bT}} d\tau_4 \int_{-\frac{1}{2bT}}^{\tau_4 - x_c} d\tau_3 \int_{-\frac{1}{2bT}}^{\tau_3 - x_c} d\tau_2 \exp \left(-\gamma^2 \ln \left(\frac{\tau_4 - \tau_3}{x_c} \right) - \frac{\gamma^2 x_c}{\tau_4 - \tau_2} + \frac{\gamma^2 x_c}{\tau_3 - \tau_2} + \mathcal{O}(x_c^2) \right) \end{aligned} \quad (\text{D20})$$

Since this term is proportional to $d\ell$, we can omit all the b factors elsewhere. We relabel $\tau_{3,4}$ as $\tau_{1,2}$, respectively, and τ_2 as $\tau' + \frac{1}{2}x_c$:

$$\delta Z_{4,1}^{(2,1)} = \frac{\lambda_x^2}{x_c^2} \cdot \lambda_x^2 d\ell \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 \int_{-\frac{1}{2T}}^{\tau_1 - \frac{3}{2}x_c} d\tau' e^{-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right)} \left(\frac{1}{x_c} - \frac{\gamma^2}{\tau_2 - \tau'} + \frac{\gamma^2}{\tau_1 - \tau'} + \mathcal{O}(x_c) \right). \quad (\text{D21})$$

The second and third terms in the parentheses can be viewed as the interaction between charges at $\tau_{1,2}$ and the dipole at $\tau' < \tau_1$. After integrating out the dipole, we obtain

$$\delta Z_{4,1}^{(2,1)} = \frac{\lambda_x^2}{x_c^2} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 e^{-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right)} \cdot \lambda_x^2 d\ell \left[\frac{1}{x_c} \left(\frac{1}{2T} + \tau_1 - \frac{3}{2}x_c \right) + \gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{\frac{3}{2}x_c}\right) + \mathcal{O}(x_c) \right]. \quad (\text{D22})$$

We have omitted the term $\gamma^2 \ln\left(\frac{\frac{1}{2T} + \tau_1}{\frac{1}{2T} + \tau_2}\right)$ because it vanishes in the $T \rightarrow 0^+$ limit. Similarly, $\delta Z_{4,1}^{(3,2)}$ and $\delta Z_{4,1}^{(4,3)}$ are given by

$$\begin{aligned} \delta Z_{4,1}^{(3,2)} &= \frac{\lambda_x^2}{x_c^2} \cdot \frac{\lambda_x^2 d\ell}{x_c} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - 3x_c} d\tau_1 \int_{\tau_1 + \frac{3}{2}x_c}^{\tau_2 - \frac{3}{2}x_c} d\tau' \exp \left[-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right) + \gamma^2 \ln\left(\frac{\tau_2 - \tau' + \frac{1}{2}x_c}{\tau_2 - \tau' - \frac{1}{2}x_c}\right) \right. \\ &\quad \left. + \gamma^2 \ln\left(\frac{\tau' - \tau_1 + \frac{1}{2}x_c}{\tau' - \tau_1 - \frac{1}{2}x_c}\right) + \mathcal{O}(x_c^2) \right] \\ &= \frac{\lambda_x^2}{x_c^2} \cdot \frac{\lambda_x^2 d\ell}{x_c} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - 3x_c} d\tau_1 \int_{\tau_1 + \frac{3}{2}x_c}^{\tau_2 - \frac{3}{2}x_c} d\tau' e^{-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right)} \left(1 + \frac{\gamma^2 x_c}{\tau_2 - \tau'} + \frac{\gamma^2 x_c}{\tau' - \tau_1} + \mathcal{O}(x_c^2) \right) \\ &= \frac{\lambda_x^2}{x_c^2} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - 3x_c} d\tau_1 e^{-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right)} \cdot \lambda_x^2 d\ell \left(\frac{1}{x_c} (\tau_2 - \tau_1 + 3x_c) + 2\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{\frac{3}{2}x_c}\right) + \mathcal{O}(x_c) \right) \end{aligned} \quad (\text{D23})$$

and

$$\begin{aligned} \delta Z_{4,1}^{(4,3)} &= \frac{\lambda_x^2}{x_c^2} \cdot \frac{\lambda_x^2 d\ell}{x_c} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 \int_{\tau_2 + \frac{3}{2}x_c}^{\frac{1}{2T}} d\tau' \exp \left[-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right) + \gamma^2 \ln\left(\frac{\tau' - \tau_2 + \frac{1}{2}x_c}{\tau' - \tau_2 - \frac{1}{2}x_c}\right) \right. \\ &\quad \left. + \gamma^2 \ln\left(\frac{\tau' - \tau_1 - \frac{1}{2}x_c}{\tau' - \tau_1 + \frac{1}{2}x_c}\right) + \mathcal{O}(x_c^2) \right] \\ &= \frac{\lambda_x^2}{x_c^2} \cdot \frac{\lambda_x^2 d\ell}{x_c} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 \int_{\tau_2 + \frac{3}{2}x_c}^{\frac{1}{2T}} d\tau' e^{-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right)} \left(1 + \frac{\gamma^2 x_c}{\tau' - \tau_2} - \frac{\gamma^2 x_c}{\tau' - \tau_1} + \mathcal{O}(x_c^2) \right) \\ &= \frac{\lambda_x^2}{x_c^2} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 e^{-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right)} \cdot \lambda_x^2 d\ell \left(\frac{1}{x_c} \left(\frac{1}{2T} - \tau_2 - \frac{3}{2}x_c \right) + \gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{\frac{3}{2}x_c}\right) + \mathcal{O}(x_c) \right). \end{aligned} \quad (\text{D24})$$

Notice that in $\delta Z_{4,1}^{(3,2)}$ the least distance between τ_2 and τ_1 is $3x_c$. We manually change the least distance back to x_c , which will lead to an error of the same order as an $\mathcal{O}(1)$ term in the parentheses. Adding up the three terms, we obtain the total $\delta Z_{4,1}$

$$\delta Z_{4,1} = \frac{\lambda_x^2}{x_c^2} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 e^{-\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right)} \cdot \lambda_x^2 d\ell \left(\frac{1}{x_c T} + 4\gamma^2 \ln\left(\frac{\tau_2 - \tau_1}{x_c}\right) + \mathcal{O}(1) \right). \quad (\text{D25})$$

According to Eq. (D18), the renormalized two-particle partition function is $\delta Z'_2 = \delta Z_{2,0} + \delta Z_{4,1} - \delta Z_{2,1} \delta Z_{2,0}$, where $\delta Z_{2,0}$ is rescaled as explained after Eq. (D15) and $\delta Z_{2,1} = \frac{\lambda_x^2}{x_c T}$ is given in Eq. (D19). The $\frac{1}{x_c T}$ term in $\delta Z_{4,1}$ is exactly canceled by $\delta Z_{2,1} \delta Z_{2,0}$. Thus,

$$\delta Z'_2 = \frac{\lambda_x^2 e^{d\ell(2-\nu)}}{x_c^2} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 e^{-\gamma^2 \ln\left(\frac{\tau_1 - \tau_2}{x_c}\right)} \cdot \left(1 + 4\gamma^2 \lambda_x^2 d\ell \cdot \ln\left(\frac{\tau_1 - \tau_2}{x_c}\right) + \mathcal{O}(\lambda_x^2 d\ell \cdot 1) \right) + \mathcal{O}(d\ell^2) + \mathcal{O}(\lambda_x^6). \quad (\text{D26})$$

Comparing it to the original form of the partition function in Eq. (D11), one can immediately read the renormalizations to parameters

$$\lambda_x^2(\ell + d\ell) = \lambda_x^2(\ell) e^{d\ell(2-\gamma^2)}, \quad \gamma^2(\ell + d\ell) = \gamma^2(\ell) - 4\gamma^2(\ell) \cdot \lambda_x^2 \cdot d\ell. \quad (\text{D27})$$

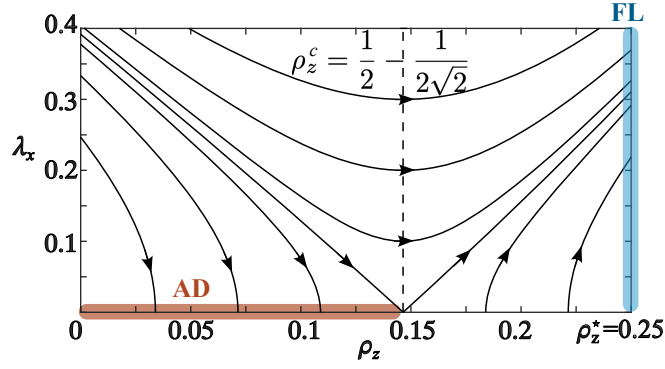


FIG. 7. RG flow of the pair-Kondo model.

The omitted $\mathcal{O}(\lambda_x^2 d\ell \cdot 1)$ term will lead to an $\mathcal{O}(\lambda_x^4)$ correction to λ_x^2 . Recall $\gamma = 2 - 4\rho_z$, we derive the flow equations

$$\frac{d\lambda_x}{d\ell} = \left(1 - \frac{\gamma^2}{2}\right) \lambda_x + \mathcal{O}(\lambda_x^3) = (-1 + 8\rho_z - 8\rho_z^2) \lambda_x + \mathcal{O}(\lambda_x^3), \quad (\text{D28})$$

$$\frac{d\rho_z}{d\ell} = (1 - 2\rho_z) \lambda_x^2 + \mathcal{O}(\lambda_x^3). \quad (\text{D29})$$

We will omit the $\mathcal{O}(\lambda_x^3)$ terms.

3. Phase diagram and a BKT transition

Phase diagram—To simplify the calculation, we want to find an invariant that is unchanged under the flow. We observe

$$d\ell = \frac{d\lambda_x}{(1 - \gamma^2/2)\lambda_x} = -\frac{d\gamma^2}{4\gamma^2\lambda_x^2} \quad \Rightarrow \quad 4\lambda_x d\lambda_x = \left(-\frac{1}{\gamma^2} + \frac{1}{2}\right) d\gamma^2. \quad (\text{D30})$$

Integrating both sides, we obtain the invariant

$$c = \lambda_x^2 + \ln \gamma - \frac{\gamma^2}{4} + \frac{1 - \ln 2}{2} = \lambda_x^2 + \ln(1 - 2\rho_z) - (1 - 2\rho_z)^2 + \frac{1 + \ln 2}{2} \quad (\text{D31})$$

up to a constant. A given c value defines a curve in the ρ_z - λ_x plane, and the flow flows these curves. We hence obtain the flow diagram in Fig. 7.

There are two types of stable fixed lines: the blue one at $\rho_z^* = \frac{1}{4}$ and the red one at $\lambda_x = 0, \rho_z < \frac{1}{2} - \frac{1}{2\sqrt{2}}$. We have chosen convention that $c = 0$ at the critical point $\lambda_x = 0, \rho_z = \frac{1}{2} - \frac{1}{2\sqrt{2}}$. The red fixed line corresponds to the anisotropic local doublet phase discussed in the last section. However, the flow in Eqs. (D28) and (D29) seems not stop at the blue fixed point. This is due to the invalidity of the perturbation theory (Eq. (D14)) around the strong coupling line. As will be clear soon, the low-energy physics at $\rho_z^* = \frac{1}{4}$ is equivalent to a free-fermion system with a phase shift. Thus, $\rho_z^* = \frac{1}{4}$ represents a free-fermion fixed point. A straightforward analysis shows the phases diagram:

$$\text{Kondo Fermi liquid:} \quad c > 0 \quad \text{or} \quad \rho_z > \frac{1}{2} - \frac{1}{2\sqrt{2}}, \quad (\text{D32})$$

$$\text{anisotropic local doublet:} \quad c < 0 \quad \text{and} \quad \rho_z < \frac{1}{2} - \frac{1}{2\sqrt{2}}. \quad (\text{D33})$$

Expression of Kondo temperature— c is the controlling parameter for the phase transition. If $c = 0$, the RG flow will take an infinite RG time ($\ell \rightarrow \infty$) to achieve the critical point at $\lambda_x = 0, \rho_z = \frac{1}{2} - \frac{1}{2\sqrt{2}}$. This is because the flow velocity approaches zero at the critical point. If c is positive but small, the renormalized parameters will eventually hit the Fermi liquid fixed line, but

the flow is extremely slow around the critical point at $\lambda_x = 0$, $\rho_z = \frac{1}{2} - \frac{1}{2\sqrt{2}}$. Thus, to estimate the RG time it takes to achieve the Fermi liquid fixed line, it suffices to examine the flow equations around the critical point:

$$\frac{d\lambda_x}{d\ell} = t\lambda_x, \quad \frac{dt}{d\ell} = 4\lambda_x^2, \quad (\text{D34})$$

where $t = 1 - \gamma^2/2 = -1 + 8\rho_z - 8\rho_z^2$ and only quadratic and bilinear terms in t and λ_x are kept. To the same order, $c = \lambda_x^2 - \frac{1}{4}t^2$. The flow equation for t is

$$\frac{dt}{d\ell} = 4c + t^2. \quad (\text{D35})$$

Since c is invariant under the flow, we have the solution

$$\ell = \ell_0 + \frac{1}{\sqrt{4c}} \arctan \frac{t}{\sqrt{4c}}. \quad (\text{D36})$$

Here ℓ_0 is the initial RG time for the energy scale D_{PK} where the pair-Kondo model is justified. The Fermi liquid fixed line is characterized by $t = \frac{1}{2}$ ($\gamma = 1$, $\rho_z = \rho_z^* = \frac{1}{4}$). Given c being small, $t/\sqrt{4c} \rightarrow \infty$, the RG time from the energy scale D_{PK} to the Kondo temperature is $\ell - \ell_0 \approx \frac{\pi}{4\sqrt{c}}$. Therefore, the Kondo temperature is determined as

$$T_K \sim D_{\text{PK}} \cdot \exp\left(-\frac{\pi}{4\sqrt{c}}\right), \quad (1 \gg c > 0). \quad (\text{D37})$$

E. Exact solution to the pair-Kondo model at $\rho_z^* = \frac{1}{4}$

In this section we use the refermionization technique [101–103] to calculate the finite-size many-body spectrum and various correlation functions of the pair-Kondo Hamiltonian (Eq. (B39)) at the strong coupling fixed line $\rho_z^* = \frac{1}{4}$.

1. Refermionization

At the fixed line $\rho_z^* = \frac{1}{4}$, the pair-Kondo Hamiltonian $\bar{H}_{\text{PK}} = U H_{\text{PK}} U^\dagger$ (Eq. (B39)) reads

$$\begin{aligned} \bar{H}_{\text{PK}} = \sum_{\chi} \int \frac{dx}{4\pi} : (\partial_x \phi_{\chi}(x))^2 : + \frac{2\pi}{L} \left(N_c(1 - P_{\text{bc}}) + \frac{N_v \Lambda_z}{2} + \sum_{\chi} \frac{N_{\chi}^2}{2} \right) \\ + \frac{\lambda_x}{x_c} \left(\Lambda_+ F_v \cdot e^{-i\phi_v(0)} + \Lambda_- F_v^\dagger \cdot e^{i\phi_v(0)} \right). \end{aligned} \quad (\text{E1})$$

Recall that $U = e^{2i\rho_z^* \Lambda_z \phi_v(0)}$ is the gauge transformation that decouples Λ_z and $\partial_x \phi_v$, $\chi = c, v, s, vs$, and the kinetic term $\int \frac{dx}{4\pi} : (\partial_x \phi_{\chi})^2 :$ can be equivalently written as $\sum_{q>0} q b_{\chi}^\dagger(q) b_{\chi}(q)$. We have omitted the constant term $-\frac{4\rho_z^*}{x_c}(1 - \frac{\pi}{L}x_c)$ that does not affect the dynamics of the system. We have kept the $\mathcal{O}(L^{-1})$ terms in order to calculate finite-size many-body spectrum.

Since $e^{-i\phi_v(0)}$ has the same scaling dimension as a fermion operator, we will construct the pseudo-fermion $\psi_v \sim \frac{F_v}{\sqrt{2\pi x_c}} e^{-i\phi_v}$ later. For the Hamiltonian to respect fermion parity, we need to map $\Lambda_{\pm}$ to a local fermion operator. However, Λ_+ does not anti-commute with $\frac{F_v}{\sqrt{2\pi x_c}} e^{-i\phi_v(0)}$ as required for a fermion operator. To achieve the anti-commutation, we introduce a further gauge transformation $U_2 = e^{i\frac{\pi}{4} N_v \Lambda_z}$. It rotates Λ_+ and F_v to

$$U_2 \cdot \Lambda_+ \cdot U_2^\dagger = e^{i\frac{\pi}{2} N_v} \cdot \Lambda_+, \quad U_2 \cdot F_v \cdot U_2^\dagger = e^{-i\frac{\pi}{2} \Lambda_z} \cdot F_v \quad (\text{E2})$$

respectively, where we have exploited Eq. (A36) and $[\Lambda_z, \Lambda_+] = 2\Lambda_+$, $[N_v, F_v] = -2F_v$. Then we have the further transformed Hamiltonian $\hat{H}_{\text{PK}} = U_2 \bar{H}_{\text{PK}} U_2^\dagger$,

$$\hat{H}_{\text{PK}} = \sum_{\chi} \int \frac{dx}{4\pi} : (\partial_x \phi_{\chi}(x))^2 : + \frac{2\pi}{L} \left(N_c(1 - P_{\text{bc}}) + \frac{N_v \Lambda_z}{2} + \sum_{\chi} \frac{N_{\chi}^2}{2} \right) + \frac{\lambda_x}{x_c} \left(f_v^\dagger F_v \cdot e^{-i\phi_v(0)} + h.c. \right), \quad (\text{E3})$$

where local fermion operators

$$f_v^\dagger = e^{i\frac{\pi}{2} N_v} \cdot \Lambda_+ \cdot e^{-i\frac{\pi}{2} \Lambda_z}, \quad f_v = e^{-i\frac{\pi}{2} N_v} \cdot e^{i\frac{\pi}{2} \Lambda_z} \cdot \Lambda_- \quad (\text{E4})$$

are introduced. They satisfy the canonical anti-commutation relation, *i.e.*, $\{f_v, f_v^\dagger\} = 1$, and

$$f_v^\dagger f_v = \frac{\Lambda_z + \Lambda_0}{2}, \quad f_v f_v^\dagger = \frac{\Lambda_0 - \Lambda_z}{2}. \quad (\text{E5})$$

Due to the $e^{\pm i\frac{\pi}{2} N_v}$ factor, they also anti-commute with the composite Klein factor F_v :

$$\{f_v, F_v\} = \{f_v^\dagger, F_v\} = \{f_v, F_v^\dagger\} = \{f_v^\dagger, F_v^\dagger\} = 0. \quad (\text{E6})$$

One may attempt to construct the pseudo-fermion as $\psi_v(x) = \frac{F_v}{\sqrt{2\pi x_c}} e^{-i\phi_v(x)} e^{-i(N_v - \frac{P'_{\text{bc}}}{2}) \frac{2\pi}{L} x}$ in analog to Eq. (A6), where N_v plays the role of the total charge of pseudo-fermions, and P'_{bc} determines the boundary condition. But this construction is invalid because F_v changes N_v by -2 rather than -1 , which is crucial for the anti-commutation relations such as $\{\psi_v(x), \psi_v(x')\} = 0$. (See calculations around Eq. (A18) for more details.) In order to resolve this issue, we introduce a new basis for particle numbers

$$\begin{bmatrix} \mathcal{N}_v \\ \mathcal{N}_1 \\ \mathcal{N}_2 \\ \mathcal{N}_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} N_{+\uparrow} \\ N_{+\downarrow} \\ N_{-\uparrow} \\ N_{-\downarrow} \end{bmatrix} \quad (\text{E7})$$

which satisfy

$$[F_v, \mathcal{N}_v] = F_v, \quad [F_v, \mathcal{N}_{1,2,3}] = 0. \quad (\text{E8})$$

We can express N_{ls} and N_χ in terms of $\mathcal{N}$'s as

$$\begin{bmatrix} N_{+\uparrow} \\ N_{+\downarrow} \\ N_{-\uparrow} \\ N_{-\downarrow} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mathcal{N}_v \\ \mathcal{N}_1 \\ \mathcal{N}_2 \\ \mathcal{N}_3 \end{bmatrix}, \quad \begin{bmatrix} N_c \\ N_v \\ N_s \\ N_{vs} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & 1 & 1 & 1 \\ 4 & 1 & -1 & -1 \\ 0 & -1 & 1 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} \mathcal{N}_v \\ \mathcal{N}_1 \\ \mathcal{N}_2 \\ \mathcal{N}_3 \end{bmatrix}. \quad (\text{E9})$$

Note that the transformations between $N_{\alpha s}$ and $\mathcal{N}$ are unimodular, meaning that *any integer-valued* $\mathcal{N}$ are physical. Therefore, we define the pseudo-fermion operator as

$$\psi_v(x) = \frac{F_v}{\sqrt{2\pi x_c}} \cdot e^{-i(\mathcal{N}_v - \frac{1}{2})\frac{2\pi x}{L}} \cdot e^{-i\phi_v(x)}. \quad (\text{E10})$$

Since P'_{bc} is independent to the physical boundary condition P_{bc} and is just a gauge choice, we have chosen $P'_{bc} = 1$ for simplicity. We also introduce the Fourier decomposition

$$\psi_v(x) = \sqrt{\frac{1}{L}} \sum_k d_v(k) e^{-ikx}, \quad k \in \frac{2\pi}{L} \left(\mathbb{Z} - \frac{1}{2} \right). \quad (\text{E11})$$

Following the calculations in Sec. A 1, there are

$$\{\psi_v(x), \psi_v(x')\} = 0, \quad \{\psi_v(x), \psi_v^\dagger(x')\} = \delta(x - x') \quad (\text{E12})$$

$$[d_v(k), \mathcal{N}_v] = c_{k,v}, \quad \{d_v(k), d_v(k')\} = 0, \quad \{d_v(k), d_v^\dagger(k')\} = \delta_{k,k'}. \quad (\text{E13})$$

Since $f_v^{(\dagger)}$ anti-commute with $F_v^{(\dagger)}$, they anti-commute with $\psi_v^{(\dagger)}$ and $d_v^{(\dagger)}(k)$ as well.

The many body Hilbert space is completely indexed by the integers

$$\{\mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_3, b_c^\dagger(q)b_c(q), b_s^\dagger(q)b_s(q), b_{vs}^\dagger(q)b_{vs}(q), f_v^\dagger f_v, d_v^\dagger(k)d_v(k)\}. \quad (\text{E14})$$

We define an auxiliary vacuum state as the Fock state $|\Omega'_0\rangle$ satisfying

$$\langle \Omega'_0 | f_v^\dagger f_v | \Omega'_0 \rangle = 0, \quad \langle \Omega'_0 | d_v^\dagger(k) d_v(k) | \Omega'_0 \rangle = \theta(k < 0), \quad (\text{E15})$$

where $k \in \frac{2\pi}{L}(\mathbb{Z} - \frac{1}{2})$. Note that $|\Omega'_0\rangle$ may not be the ground state even in the absence of λ_x . $\mathcal{N}_v$ is not an independent quantum number because

$$\mathcal{N}_v = \sum_k : d_v^\dagger(k) d_v(k) : \quad (\text{E16})$$

where the normal ordering respects $|\Omega'_0\rangle$.

Referring to Eq. (A26), the Hamiltonian term $\int \frac{dx}{4\pi} : (\partial_x \phi_v)^2 :$ can be expressed in terms of d_v and $\mathcal{N}_v$ as

$$\int \frac{dx}{4\pi} : (\partial_x \phi_v(x))^2 : = \sum_{k \in \frac{2\pi}{L}(\mathbb{Z} - \frac{1}{2})} k : d_v^\dagger(k) d_v(k) : - \frac{2\pi}{L} \frac{\mathcal{N}_v^2}{2}. \quad (\text{E17})$$

The normal ordering on the left-hand side respects $|0\rangle_0$ in the original representation, and the normal ordering on the right-hand side respects $|\Omega'_0\rangle$ in the pseudo-fermion representation. Since the two hand sides only differ by a constant if $|\Omega'_0\rangle \neq |0\rangle_0$, we do not attempt to identify the relation between the two vacuum states. The Hamiltonian $\hat{H}_{PK}$ becomes

$$\begin{aligned} \hat{H}_{PK} = & \frac{2\pi}{L} \frac{(\mathcal{N}_1 + \mathcal{N}_2 + \mathcal{N}_3)(1 - P_{bc})}{2} + \frac{2\pi}{L} \cdot \frac{1}{2} (\mathcal{N}_v \mathcal{N}_1 \mathcal{N}_2 \mathcal{N}_3) \begin{bmatrix} 3 & 1 & -1 & -1 \\ 1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} \mathcal{N}_v \\ \mathcal{N}_1 \\ \mathcal{N}_2 \\ \mathcal{N}_3 \end{pmatrix} + \sum_{\chi=c,s,vs} \sum_q q b_\chi^\dagger(q) b_\chi(q) \\ & + \frac{2\pi}{L} N_v \left(f_v^\dagger f_v - \frac{1}{2} \right) + \sum_{k \in \frac{2\pi}{L}(\mathbb{Z} - \frac{1}{2})} k : d_v^\dagger(k) d_v(k) : + \lambda_x \sqrt{\frac{2\pi}{x_c L}} \sum_k (f_v^\dagger d_v(k) + d_v^\dagger(k) f_v(k)), \end{aligned} \quad (\text{E18})$$

where we have used the transformation Eq. (E9) and $\frac{\Lambda_z}{2} = f_v^\dagger f_v - \frac{1}{2}$. The above equation is almost a free-fermion problem. The only subtlety is that $\mathcal{N}_v$ in the first row and N_v in the second row do not commute with the hopping term $f_v^\dagger d_v$. To resolve this issue, we introduce the total pseudo-fermion charge

$$\mathcal{N}_{\text{pf}} = f_v^\dagger f_v + \mathcal{N}_v = f_v^\dagger f_v + \sum_k : d_v^\dagger(k) d_v(k) : \quad (\text{E19})$$

which is conserved by the Hamiltonian, and express N_v and $\mathcal{N}_v$ in terms of $\mathcal{N}_{\text{pf}}$, $f_v^\dagger f_v$, and $\mathcal{N}_{1,2,3}$:

$$\mathcal{N}_v = \mathcal{N}_{\text{pf}} - f_v^\dagger f_v, \quad N_v = 2\mathcal{N}_{\text{pf}} - 2f_v^\dagger f_v + \frac{1}{2} (\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3) . \quad (\text{E20})$$

Then, we rewrite the terms involving N_v or $\mathcal{N}_v$ in the Hamiltonian as

$$N_v \left(f_v^\dagger f_v - \frac{1}{2} \right) = \left(2\mathcal{N}_{\text{pf}} + \frac{1}{2} [\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] - 1 \right) f_v^\dagger f_v - \mathcal{N}_{\text{pf}} - \frac{1}{4} [\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] \quad (\text{E21})$$

$$\mathcal{N}_v (\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3) = \mathcal{N}_{\text{pf}} (\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3) - (\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3) f_v^\dagger f_v \quad (\text{E22})$$

$$\frac{3}{2} \mathcal{N}_v^2 = \frac{3}{2} \mathcal{N}_{\text{pf}}^2 + \left(\frac{3}{2} - 3\mathcal{N}_{\text{pf}} \right) f_v^\dagger f_v , \quad (\text{E23})$$

where we have used $(f_v^\dagger f_v)^2 = f_v^\dagger f_v$. Substituting these relations into the Hamiltonian gives

$$\begin{aligned} \hat{H}_{\text{PK}} = & \frac{2\pi}{L} \left(\sum_{i=1}^3 \left[\frac{(1 - P_{\text{bc}})}{2} \mathcal{N}_i + \frac{\mathcal{N}_i^2}{2} \right] - \mathcal{N}_{\text{pf}} - \frac{1}{4} [\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] + \mathcal{N}_{\text{pf}} \left[\frac{3}{2} \mathcal{N}_{\text{pf}} + \mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3 \right] \right) \\ & + \sum_{\chi=c,s,vs} \sum_q q b_\chi^\dagger(q) b_\chi(q) \\ & + \varepsilon_f f_v^\dagger f_v + \sum_{k \in \frac{2\pi}{L}(\mathbb{Z} - \frac{1}{2})} k : d_v^\dagger(k) d_v(k) : + \sqrt{\frac{2\pi\Gamma}{L}} \sum_{k \in \frac{2\pi}{L}(\mathbb{Z} - \frac{1}{2})} (f_v^\dagger d_v(k) + d_v^\dagger(k) f_v) , \end{aligned} \quad (\text{E24})$$

where

$$\varepsilon_f = \frac{2\pi}{L} \left(\frac{1}{2} - \mathcal{N}_{\text{pf}} - \frac{1}{2} [\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] \right), \quad \Gamma = \frac{\lambda_x^2}{x_c}, \quad (\text{E25})$$

the normal ordering respects $|\Omega'_0\rangle$.

As an independent check, we numerically compare the referminized $\hat{H}_{\text{PK}}$ (Eq. (E24)) to $\bar{H}_{\text{PK}}$ (Eq. (E1)) in the $\lambda_x = 0$ limit in the quantum number sector $b_\chi^\dagger(q) b_\chi(q) = 0$ ($\chi = c, v, s, vs$). In this limit, the energy of $\bar{H}_{\text{PK}}$ in Eq. (E1) is fully determined by N_{ls} and Λ_z . Given N_{ls} and Λ_z , one can further determine $\mathcal{N}_{\text{ps}}$, $\mathcal{N}_{1,2,3}$, $f_v^\dagger f_v$, and then calculate the energy using $\hat{H}_{\text{PK}}$, where $\sum_k k : d_v^\dagger(k) d_v(k) :$ should take its lowest value $\frac{2\pi}{L} \frac{1}{2} (\mathcal{N}_{\text{pf}} - f_v^\dagger f_v)^2$ according to Eq. (E17). Numerical calculations confirm that the two Hamiltonians always yield identical energies.

Now we are ready to diagonalize $\hat{H}_{\text{PK}}$. We first enumerate the conserved quantum numbers $\mathcal{N}_{\text{pf}}$, $\mathcal{N}_{1,2,3}$, $b_\chi^\dagger(q) b_\chi(q)$ ($\chi = c, s, vs$), which take values in integers. For a given set of quantum numbers, $\hat{H}_{\text{PK}}$ is a free-fermion Hamiltonian in the Hilbert space spanned by f_v and $d_v(k)$, and its many-body eigenstates are just Fock states of the eigenmodes of the hopping Hamiltonian. These states live in an *extended* Hilbert space indexed by

$$\{ \mathcal{N}_{\text{pf}}, \mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_3, b_c^\dagger(q) b_c(q), b_s^\dagger(q) b_s(q), b_{vs}^\dagger(q) b_{vs}(q), f_v^\dagger f_v, d_v^\dagger(k) d_v(k) \} . \quad (\text{E26})$$

Not all states are physical because $\mathcal{N}_{\text{pf}}$ should equal to $f_v^\dagger f_v + \sum_k : d_v^\dagger(k) d_v(k) :$ (Eq. (E19)). Therefore, we should discard states violating this constraint in the end.

For later convenience, we define the vacuum state in the *extended* Hilbert space for given quantum numbers $\mathcal{N}_{\text{pf},1,2,3}$ as

$$\langle \Omega_0 | f_v^\dagger f_v | \Omega_0 \rangle = \theta(\varepsilon_f \leq 0), \quad \langle \Omega_0 | d_v^\dagger(k) d_v(k) | \Omega_0 \rangle = \theta(k < 0) . \quad (\text{E27})$$

Note that $|\Omega_0\rangle$ is the ground state in the sector of quantum numbers $\mathcal{N}_{\text{pf},1,2,3}$ if $\lambda_x = 0$, and it is not necessarily physical. Then we rewrite $\hat{H}_{\text{PK}}$ as

$$\begin{aligned} \hat{H}_{\text{PK}} = & \frac{2\pi}{L} \left(\sum_{i=1}^3 \left[\frac{(1-P_{\text{bc}})}{2} \mathcal{N}_i + \frac{\mathcal{N}_i^2}{2} \right] - \mathcal{N}_{\text{pf}} - \frac{1}{4} [\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] + \mathcal{N}_{\text{pf}} \left[\frac{3}{2} \mathcal{N}_{\text{pf}} + \mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3 \right] \right) \\ & + \sum_{\chi=c,s,vs} \sum_q q b_\chi^\dagger(q) b_\chi(q) + \theta(\varepsilon_f \leq 0) \varepsilon_f \\ & + \varepsilon_f : f_v^\dagger f_v : + \sum_{k \in \frac{2\pi}{L}(\mathbb{Z} - \frac{1}{2})} k : d_v^\dagger(k) d_v(k) : + \sqrt{\frac{2\pi\Gamma}{L}} \sum_{k \in \frac{2\pi}{L}(\mathbb{Z} - \frac{1}{2})} (f_v^\dagger d_v(k) + d_v^\dagger(k) f_v) . \end{aligned} \quad (\text{E28})$$

Here the normal ordering respects $|\Omega_0\rangle$. The vacuum energy subducted in $\varepsilon_f : f_v^\dagger f_v : + \sum_k k : d_v^\dagger(k) d_v(k) :$ is

$$E[\Omega_0] = \theta(\varepsilon_f \leq 0) \cdot \varepsilon_f + \sum_{n=-\infty}^0 \frac{2\pi}{L} \left(n - \frac{1}{2} \right) . \quad (\text{E29})$$

A regularization is needed to obtain a finite value.

2. Finite-size many-body spectrum

Next, we diagonalize the hopping Hamiltonian in the third row of $\hat{H}_{\text{PK}}$ (Eq. (E28)). Suppose the eigen mode is given by $d_n^\dagger = u_n f_v^\dagger + \sum_k v_{k,n} d_v^\dagger(k)$, and the hopping Hamiltonian equals to

$$\sum_n \epsilon_n \star d_n^\dagger d_n \star + \delta E[\Omega] \quad (\text{E30})$$

where $\star \cdots \star$ is the normal ordering with respect to the vacuum state $|\Omega\rangle$ in the presence of λ_x , and $\delta E[\Omega]$ is the change of vacuum energy from $|\Omega_0\rangle$. The equation of motion is given by

$$f_v^\dagger \left(\varepsilon_f \cdot u_n + \sqrt{\frac{2\pi\Gamma}{L}} \sum_k v_{k,n} \right) + \sum_k d_v^\dagger(k) \left(k \cdot v_{k,n} + \sqrt{\frac{2\pi\Gamma}{L}} \cdot u_n \right) = f_v^\dagger \cdot \epsilon_n u_n + \sum_k d_v^\dagger(k) \cdot \epsilon_n v_{k,n} , \quad (\text{E31})$$

where the left-hand side is the commutator of the hopping Hamiltonian in $\hat{H}_{\text{PK}}$ and $d_n^\dagger$, and the right-hand side is the commutator $[\epsilon_n \star d_n^\dagger d_n \star, d_n^\dagger]$. The above equation implies

$$\epsilon_n - \varepsilon_f = \frac{2\pi\Gamma}{L} \sum_k \frac{1}{\varepsilon_n - k} = \pi\Gamma \sum_{j=-\infty}^{\infty} \frac{1}{\frac{L}{2}\varepsilon_n - \pi(j - \frac{1}{2})} = -\pi\Gamma \cdot \tan \frac{L\epsilon_n}{2} , \quad (\text{E32})$$

where we have used the Mittag-Leffler expansion, $\tan z = \sum_{j=-\infty}^{+\infty} \frac{-1}{z - \pi(j - \frac{1}{2})}$, as $\tan z$ has poles of residue -1 at $z = \pi(n - \frac{1}{2})$. For $|\epsilon_n - \varepsilon_f| \ll \Gamma$, there must be $\epsilon_n \in \frac{2\pi}{L}\mathbb{Z}$. For $|\epsilon_n - \varepsilon_f| \gg \Gamma$, there must be $\epsilon_n \in \frac{2\pi}{L}(\mathbb{Z} + \frac{1}{2})$. We denote the levels as

$$\epsilon_n = \frac{2\pi}{L} \left(n - \frac{1}{2} + \delta_n \right) , \quad \delta_n = \begin{cases} \frac{1}{\pi} \arctan \frac{\pi\Gamma}{\epsilon_n - \varepsilon_f - 0^+} , & \epsilon_n \leq \varepsilon_f \\ -1 + \frac{1}{\pi} \arctan \frac{\pi\Gamma}{\epsilon_n - \varepsilon_f} , & \epsilon_n > \varepsilon_f \end{cases} \quad (\text{E33})$$

with δ_n being the phase shift, as shown in Fig. 8. In the $\Gamma \gg \frac{2\pi}{L}$ limit, as n increases from $-\infty$ to 0, δ_n changes from 0 to $-\frac{1}{2}$. As n further increases to ∞ , δ_n decreases to -1 .

As shown in Fig. 8, no level crossing happens as Γ (or λ_x) is turned on. Thus, one can derive the ground state $|\Omega\rangle$ from $|\Omega_0\rangle$ (Eq. (E27)) by tracking the evolution of occupied levels with respect to Γ . For $\varepsilon_f \leq 0$, the highest occupied level in $|\Omega\rangle$ is ϵ_1 ; for $\varepsilon_f > 0$, the highest occupied level in $|\Omega\rangle$ is ϵ_0 . Thus, the vacuum energy subducted in the normal ordering $\sum_n \epsilon_n \star d_n^\dagger d_n \star$ is $E[\Omega] = \sum_{n=-\infty}^1 \epsilon_n$ and $\sum_{n=-\infty}^0 \epsilon_n$ for $\varepsilon_f \leq 0$ and $\varepsilon_f > 0$, respectively. Since $\epsilon_1 = 0$ in the $\Gamma \gg \frac{2\pi}{L}$ limit, we can always calculate $E[\Omega]$ as

$$E[\Omega] = \sum_{n=-\infty}^0 \frac{2\pi}{L} \left(n - \frac{1}{2} + \delta_n \right) . \quad (\text{E34})$$

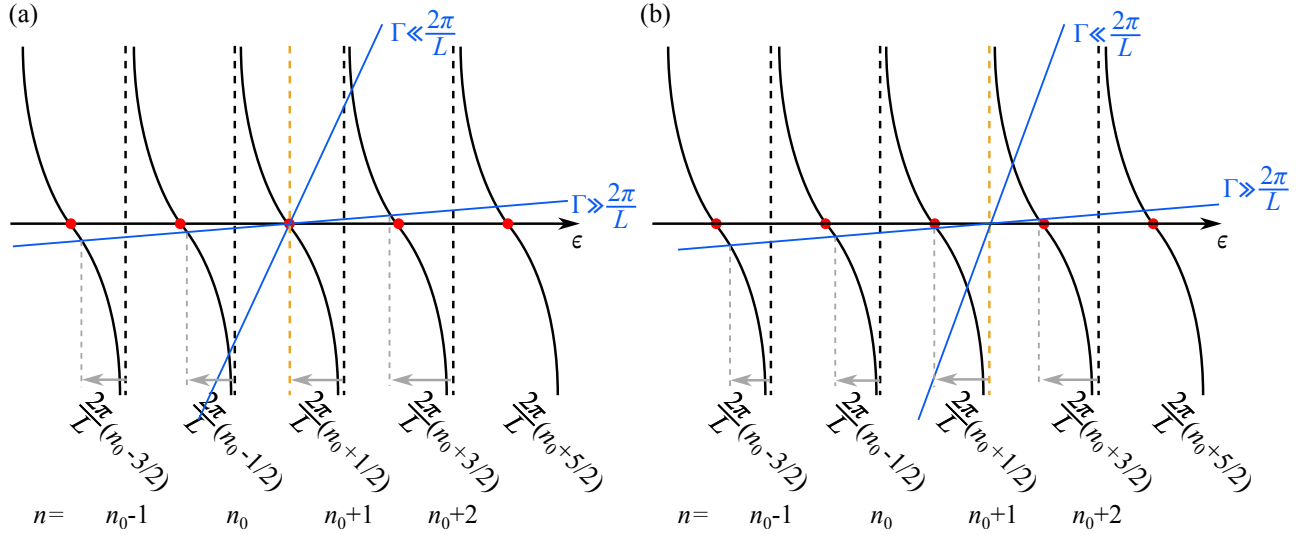


FIG. 8. Phase shift of energy levels of the pair-Kondo model at the Fermi liquid fixed point $\rho^* = \frac{1}{4}$. Black vertical dashed lines indicate $\epsilon = \frac{2\pi}{L} (n - \frac{1}{2})$ ($n \in \mathbb{Z}$), and yellow vertical dashed lines represent ϵ_f , which is $\frac{2\pi}{L} n_0$ and $\frac{2\pi}{L} (n_0 + \frac{1}{2})$ in (a) and (b), respectively. Red dots indicate $\epsilon = \frac{2\pi}{L} n$. The blue lines are $\frac{\epsilon - \epsilon_f}{\Gamma}$. The black curves are the function $-\tan(\frac{\epsilon}{2})$, their crossings with the blue lines give the eigenvalues $\epsilon_n = \frac{2\pi}{L} (n - \frac{1}{2} + \delta_n)$. $\frac{2\pi}{L} \delta_n$ is shown by the gray arrows.

Comparing it to Eq. (E29), we have the correction to vacuum energy as

$$\delta E[\Omega] = E[\Omega] - E[\Omega_0] = -\theta(\epsilon_f \leq 0) \cdot \epsilon_f + \sum_{n=-N}^0 \frac{2\pi}{L} \delta_n = -\theta(\epsilon_f \leq 0) \cdot \epsilon_f + \delta E'[\Omega]. \quad (\text{E35})$$

We need to evaluate the second term $\delta E'[\Omega]$. Notice

$$\begin{aligned} \frac{2\pi}{L} \delta_n &= \frac{2}{L} \arctan \frac{\pi\Gamma}{\frac{2\pi}{L}(n - \frac{1}{2}) - \epsilon_f - 0^+} - \frac{2\pi}{L} \cdot \theta\left(\frac{2\pi}{L} \left[n - \frac{1}{2}\right] > \epsilon_f\right) \\ &\quad - \left(\frac{2\pi}{L}\right)^2 \delta_n \cdot \left(\frac{\Gamma}{(\pi\Gamma)^2 + (\frac{2\pi}{L}(n - \frac{1}{2}) - \epsilon_f)^2} + \delta\left(\frac{2\pi}{L} \left[n - \frac{1}{2}\right] - \epsilon_f\right) \right) + \mathcal{O}(L^{-3}) \end{aligned} \quad (\text{E36})$$

The first term in the second row is of the order $\mathcal{O}(L^{-2})$. After summing over $N \sim L$ terms, they contribute to an $\mathcal{O}(L^{-1})$ term to $\delta E'[\Omega]$. However, the contribution to $\delta E'[\Omega]$ from the ϵ_f -dependent part of these terms is of the order $\mathcal{O}(L^{-2})$. Since our focus is on the ϵ_f -dependent $\mathcal{O}(L^{-1})$ terms in $\delta E'[\Omega]$, and constant $\mathcal{O}(L^{-1})$ terms are irrelevant, we can neglect the second row of the above equation. We can replace the first row in the above equation by the integral $\int_{n-1}^n dx f(x) + \mathcal{O}(f''(n - \frac{1}{2}))$, where

$$f(x) = \frac{2}{L} \arctan \frac{\pi\Gamma}{\frac{2\pi}{L}x - \epsilon_f} - \frac{2\pi}{L} \theta\left(\frac{2\pi}{L}x - \epsilon_f\right) \quad (\text{E37})$$

The $\mathcal{O}(f''(n - \frac{1}{2}))$ term is of the order $\mathcal{O}(L^{-3})$ and eventually leads to an $\mathcal{O}(L^{-2})$ term in $\delta E'[\Omega]$. We hence can safely omit the $\mathcal{O}(f''(n - \frac{1}{2}))$ term. It is worth mentioning that the integral expression also applies when $\frac{2\pi}{L}(n - \frac{1}{2}) = \epsilon_f$ if $\epsilon_f \in \frac{2\pi}{L}(\mathbb{Z} + \frac{1}{2})$. In this case, the integral reproduces $\frac{\pi}{L}$. Therefore, $\delta E'[\Omega]$ is given by the integral

$$\begin{aligned} \delta E'[\Omega] &= \theta(\epsilon_f \leq 0) \cdot \epsilon_f + \frac{2}{L} \int_{-D \frac{L}{2\pi}}^0 dx \arctan \left(\frac{\pi\Gamma}{\frac{2\pi}{L}x - \epsilon_f} \right) = \theta(\epsilon_f \leq 0) \cdot \epsilon_f + \Gamma \int_{\frac{-D - \epsilon_f}{\pi\Gamma}}^{-\frac{\epsilon_f}{\pi\Gamma}} d\epsilon \arctan \frac{1}{\epsilon} \\ &= \theta(\epsilon_f \leq 0) \cdot \epsilon_f + \Gamma \cdot \left(\frac{1}{2} \ln[\epsilon^2 + 1] + \epsilon \cdot \arctan \frac{1}{\epsilon} \right) \Big|_{\frac{-D - \epsilon_f}{\pi\Gamma}}^{-\frac{\epsilon_f}{\pi\Gamma}} \\ &= \theta(\epsilon_f \leq 0) \cdot \epsilon_f - \Gamma - \Gamma \ln \left(\frac{D}{\Gamma} \right) + \epsilon_f \cdot \frac{\arctan \frac{\pi\Gamma}{\epsilon_f}}{\pi} - \frac{\Gamma\epsilon_f}{D} + \mathcal{O}(L^{-2}) + \mathcal{O}(D^{-2}) \end{aligned}$$

$$\Gamma \gg |\varepsilon_f| \quad \frac{1}{2}\varepsilon_f - \Gamma - \Gamma \ln \left(\frac{D}{\Gamma} \right) - \frac{\Gamma \varepsilon_f}{D} + \mathcal{O}(L^{-2}) + \mathcal{O}(D^{-2}). \quad (\text{E38})$$

It is a smooth function as ε_f crosses zero. Therefore, we have

$$\delta E[\Omega] \stackrel{D \rightarrow \infty}{\approx} -\theta(\varepsilon_f \leq 0) \cdot \varepsilon_f + \frac{1}{2}\varepsilon_f - \Gamma - \Gamma \ln \left(\frac{D}{\Gamma} \right) + \dots \quad (\text{E39})$$

The omitted terms include $\mathcal{O}(L^{-1})$ terms that are independent to ε_f , $\mathcal{O}(D^{-1})$ terms, and $\mathcal{O}(L^{-2})$ terms.

Up to constant terms irrelevant in excitation energies, the Hamiltonian in Eq. (E28) equals to

$$\begin{aligned} \hat{H}_{\text{PK}} = & \frac{2\pi}{L} \left(\sum_{i=1}^3 \left[\frac{(1-P_{\text{bc}})}{2} \mathcal{N}_i + \frac{\mathcal{N}_i^2}{2} \right] - \frac{3}{2} \mathcal{N}_{\text{pf}} - \frac{1}{2} [\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] + \mathcal{N}_{\text{pf}} \left[\frac{3}{2} \mathcal{N}_{\text{pf}} + \mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3 \right] \right) \\ & + \sum_{\chi=c,s,vs} \sum_{q>0} q b_{\chi}^{\dagger}(q) b_{\chi}(q) + \sum_{n \in \mathbb{Z}} \frac{2\pi}{L} \left(n - \frac{1}{2} + \delta_n \right) \star d_n^{\dagger} d_n \star. \end{aligned} \quad (\text{E40})$$

Recall that $\mathcal{N}_{\text{pf}}, \mathcal{N}_{1,2,3}$ are integers, ε_f is given by

$$\varepsilon_f = \frac{2\pi}{L} \left(\frac{1}{2} - \mathcal{N}_{\text{pf}} - \frac{1}{2} [\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] \right), \quad (\text{E41})$$

and δ_n is given by Eq. (E33). As we have explained above Eq. (E28), $\hat{H}_{\text{PK}}$ is defined in an extended Hilbert space, and only states subject to the constraint $\mathcal{N}_{\text{pf}} = f_v^{\dagger} f_v + \sum_k : d_v^{\dagger} d_v :$ are physical. We rewrite this constraint as $\mathcal{N}_{\text{pf}} = \theta(\varepsilon_f \leq 0) + : f_v^{\dagger} f_v : + \sum_k : d_v^{\dagger} d_v :$, where the normal ordering respects $|\Omega_0\rangle$. Since no level crossing happens as Γ is turned on, the particle number of pseudo-fermions $: f_v^{\dagger} f_v : + \sum_k : d_v^{\dagger} d_v :$ equals to $\sum_n \star d_n^{\dagger} d_n \star$. Thus, the physical constraint is given by

$$\mathcal{N}_{\text{pf}} = \theta(\varepsilon_f \leq 0) + \sum_n \star d_n^{\dagger} d_n \star. \quad (\text{E42})$$

It is also worth emphasizing that the reference state $|\Omega\rangle$ used in the normal ordering occupies levels with $n \leq 1$ when $\varepsilon_f \leq 0$, and levels with $n \leq 0$ when $\varepsilon_f > 0$, as explained above Eq. (E34).

We now derive the lowest many-body state for given $\mathcal{N}_{\text{pf}}, \mathcal{N}_{1,2,3}$ in the $\Gamma \gg \frac{2\pi}{L}$ limit. To save the energy of boson fields, there must be $b_{\chi}^{\dagger}(q) b_{\chi}(q) = 0$. For the low-energy states to be physical, they must further occupy the lowest $\mathcal{N}_{\text{pf}} - \theta(\varepsilon_f \leq 0)$ pseudo-fermion levels in addition to those occupied in $|\Omega\rangle$. If $\varepsilon_f \leq 0$, $\epsilon_{n \leq 1}$ are occupied in $|\Omega\rangle$, and $\langle \Omega | \mathcal{N}_{\text{pf}} | \Omega \rangle = \theta(-\varepsilon_f \leq 0) = 1$, then the low-energy physical state must further occupy $\epsilon_2, \epsilon_3 \dots \epsilon_{\mathcal{N}_{\text{pf}}}$, leading to the excitation energy $\frac{2\pi}{L} \cdot \frac{\mathcal{N}_{\text{pf}}(\mathcal{N}_{\text{pf}}-1)}{2}$. If $\varepsilon_f > 0$, $\epsilon_{n \leq 0}$ are occupied in $|\Omega\rangle$, and $\langle \Omega | \mathcal{N}_{\text{pf}} | \Omega \rangle = \theta(-\varepsilon_f \leq 0) = 0$, then the low-energy physical state must further occupy $\epsilon_1, \epsilon_2 \dots \epsilon_{\mathcal{N}_{\text{pf}}}$, leading to the same excitation energy $\frac{2\pi}{L} \cdot \frac{\mathcal{N}_{\text{pf}}(\mathcal{N}_{\text{pf}}-1)}{2}$. Therefore, the lowest many-body energy for given $\mathcal{N}_{\text{pf}}, \mathcal{N}_{1,2,3}$ is

$$E[\mathcal{N}_{\text{pf},1,2,3}] = \frac{2\pi}{L} \left(\sum_{i=1}^3 \left[\frac{(1-P_{\text{bc}})}{2} \mathcal{N}_i + \frac{\mathcal{N}_i^2}{2} \right] - 2\mathcal{N}_{\text{pf}} - \frac{1}{2} [\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] + \mathcal{N}_{\text{pf}} [2\mathcal{N}_{\text{pf}} + \mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3] \right). \quad (\text{E43})$$

The state is non-degenerate in a sector of given $\mathcal{N}_{\text{pf},1,2,3}$ because the boson excitations and particle-hole excitations of the pseudo-fermions cost at least an energy of $\frac{2\pi}{L}$.

According to Eq. (E9), $\mathcal{N}_{\text{pf}} (= \mathcal{N}_v + f_v^{\dagger} f_v)$ and $\mathcal{N}_{1,2,3}$ fully determine the quantum numbers $N_v^{(\text{tot})}, N_{c,s,vs}$:

$$\begin{bmatrix} N_c \\ N_v^{(\text{tot})} + 1 \\ N_s \\ N_{vs} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & 1 & 1 & 1 \\ 4 & 1 & -1 & -1 \\ 0 & -1 & 1 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} \mathcal{N}_{\text{pf}} \\ \mathcal{N}_1 \\ \mathcal{N}_2 \\ \mathcal{N}_3 \end{bmatrix}, \quad (\text{E44})$$

where $N^{(\text{tot})} = N_v + \Lambda_z = 2\mathcal{N}_v + \frac{1}{2}(\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3) + 2f_v^{\dagger} f_v - 1 = 2\mathcal{N}_{\text{pf}} + \frac{1}{2}(\mathcal{N}_1 - \mathcal{N}_2 - \mathcal{N}_3) - 1$. Expanding $\mathcal{N}_{\text{pf},1,2,3}$ in terms of $N_{c,s,vs}, N_v^{(\text{tot})}$, we derive

$$E[N_{c,s,vs}, N_v^{(\text{tot})}] = \frac{2\pi}{L} \left((1-P_{\text{bc}})N_c - \frac{1}{2} + \frac{1}{2}N_v^{(\text{tot})2} + \frac{1}{2} \sum_{\chi=c,s,vs} N_{\chi}^2 \right). \quad (\text{E45})$$

For $-1 < P_{bc} < 1$, the ground state is given by $N_c = -1$, $N_s = N_{vs} = N_v^{(\text{tot})} = 0$ ($\mathcal{N}_{\text{pf}} = \mathcal{N}_1 = 1$, $\mathcal{N}_2 = \mathcal{N}_3 = 0$), and the ground state energy is $E = \frac{2\pi}{L}(P_{bc} - 1)$. We introduce $\Delta N_c = N_c + 1$, $\Delta N_s = N_s$, $\Delta N_{vs} = N_{vs}$, and $\Delta N_v = N_v^{(\text{tot})}$ as the deviation of quantum numbers from the ground state. Then the excitation energy (with respect to the ground state) is given by

$$\Delta E = \frac{2\pi}{L} \left((-P_{bc})\Delta N_c + \frac{1}{2} \sum_{\chi=c,v,s,vs} \Delta N_\chi^2 \right). \quad (\text{E46})$$

Importantly, $\Delta N_{c,v,s,vs}$ satisfy the same free-gluing condition as $N_{c,v,s,vs}$ (Eq. (B32)), since they also correspond to integer $\mathcal{N}_{\text{pf},1,2,3}$ in the same way as $N_{c,v,s,vs}$ (Eq. (E9)):

$$\begin{bmatrix} \Delta N_c \\ \Delta N_v \\ \Delta N_s \\ \Delta N_{vs} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & 1 & 1 & 1 \\ 4 & 1 & -1 & -1 \\ 0 & -1 & 1 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} \mathcal{N}_{\text{pf}} \\ \mathcal{N}_1 \\ \mathcal{N}_2 + 1 \\ \mathcal{N}_3 + 1 \end{bmatrix}. \quad (\text{E47})$$

Comparing ΔE to H_{PK} in the initial bosonized form (Eq. (B35)), we find it equivalent to the quantum number part of H_{PK} with a new boundary condition $\tilde{P}_{bc} = P_{bc} + 1$, suggesting that the Kondo screening only introduces a π phase shift.

We now prove that *the many-body spectrum below the energy scale of Γ is equivalent to a free-fermion system with a π phase shift*. Consider the boson and particle-hole excitations in $\hat{H}_{\text{PK}}$ (Eq. (E40)) for fixed $\Delta N_{c,v,s,vs}$. The boson excitations are described by $\sum_{\chi=c,s,vs} \sum_{q>0} q b_\chi^\dagger(q) b_\chi(q)$. The particle-hole excitations in $\sum_n \frac{2\pi}{L}(n-1) d_n^\dagger d_n$ with a fixed $\mathcal{N}_{\text{pf}}$ can be equivalently written as $\sum_{q>0} q : b_v^\dagger(q) b_v(q) :$ according to the bosonization dictionary (Eq. (A26)), where $b_v(q)$ is an auxiliary construction. Thus, the effective Hamiltonian

$$H_{\text{eff}} = \frac{2\pi}{L} \left((1 - \tilde{P}_{bc})\Delta N_c + \frac{1}{2} \sum_{\chi=c,v,s,vs} \Delta N_\chi^2 \right) + \sum_{\chi=c,v,s,vs} \sum_{q>0} q b_\chi^\dagger(q) b_\chi(q) \quad (\text{E48})$$

generates all many-body levels below the energy scale of Γ . It has the same form as H_{PK} (Eq. (B35)) with $\lambda_x = \rho_z = 0$ and $\tilde{P}_{bc} = P_{bc} + 1$. Therefore, we can invert the bosonization procedure in Sec. B 3 and rewrite the effective Hamiltonian as

$$H_{\text{eff}} = \sum_{ls} \sum_k k : c_{ls}^\dagger(k) c_{ls}(k) :, \quad k \in \frac{2\pi}{L} \left(\mathbb{Z} - \frac{\tilde{P}_{bc}}{2} \right). \quad (\text{E49})$$

where $c_{ls}(k)$ are fermion operators constructed from ΔN_χ and $b_\chi(q)$.

3. Thermodynamic quantities

$\hat{H}_{\text{PK}}$ describes a fermionic level f_v subject to a hybridization bath of ψ_v . In this section, we integrate out the bath fields ψ_v , and obtain an effective theory for the fermionic level f_v only (which represents the impurity doublet), from which we can derive the impurity entropy, S_{imp} , and the static susceptibility of Λ_z operator, $\chi_z(0)$.

For this purpose, let us derive the impurity free-energy F_{imp} . In the thermodynamic limit, we can neglect all the $\mathcal{O}(L^{-1})$ terms in $\hat{H}_{\text{PK}}$ (Eq. (E28)). We write the partition function of $\hat{H}_{\text{PK}}$ in terms of a path integral over Grassmann variables $f_v^\dagger(\tau)$, $f_v(\tau)$, $d_v^\dagger(k, \tau)$, $d_v(k, \tau)$, with Fourier components over fermionic Matsubara frequencies $i\omega$,

$$f_v(\tau) = \frac{1}{\sqrt{\beta}} \sum_{i\omega} f_v(i\omega) e^{-i\omega\tau} \quad d_v(k, \tau) = \frac{1}{\sqrt{\beta}} \sum_{i\omega} d_v(k, i\omega) e^{-i\omega\tau} \quad (\text{E50})$$

We will not distinguish a Grassmann variable from a fermionic operator in the notation. Since the c, s, vs bath fields are decoupled, their partition function can be simply factored out. The remaining path integral over the v fields reads

$$Z = \text{Tr}[e^{-\beta \hat{H}_{\text{PK}}}] = \int_{\mathcal{D}[f^\dagger, f, d^\dagger, d]} \exp \left[- (S_f[f^\dagger, f] + S_d[d^\dagger, d] + S_{fd}[f^\dagger, f, d^\dagger, d]) \right] \quad (\text{E51})$$

$$\text{where} \quad S_f[f^\dagger, f] = \sum_{i\omega} f_v^\dagger(i\omega) (-i\omega + h) f_v(i\omega)$$

$$S_d[d^\dagger, d] = \sum_{i\omega, k} d_v^\dagger(k, i\omega) (-i\omega + k) d_v(k, i\omega)$$

$$S_{fd}[f^\dagger, f, d^\dagger, d] = \sqrt{\frac{2\pi\Gamma}{L}} \sum_{i\omega, k} \left(d_v^\dagger(k, i\omega) f_v(i\omega) + f_v^\dagger(i\omega) d_v(k, i\omega) \right)$$

Here, we also introduce a Zeeman field $\frac{1}{2}h\Lambda_z$, which in the pseudo-fermion language corresponds to an on-site energy of f_v .

We carry out the Gaussian integrals over $\int_{\mathcal{D}[d^\dagger, d]}$ and obtain an effective action for f_v :

$$S_{\text{imp}}[f^\dagger, f] = \sum_{i\omega} f_v^\dagger(i\omega)(-i\omega + h + \Delta(i\omega))f_v(i\omega), \quad (\text{E52})$$

where

$$\Delta(i\omega) = \frac{2\pi}{L}\Gamma \sum_k \frac{1}{i\omega - k} = \Gamma \int dk \frac{1}{i\omega - k} = -i \cdot \text{sgn}(\omega) \cdot \pi\Gamma \quad (\text{E53})$$

is the hybridization function. The partition function for the impurity is hence

$$Z_{\text{imp}} = \int_{\mathcal{D}[f^\dagger, f]} e^{-S_{\text{imp}}[f^\dagger, f]} = \prod_{i\omega} (-i\omega + h - i\pi\Gamma \cdot \text{sgn}(\omega)). \quad (\text{E54})$$

The free-energy is hence given by

$$\begin{aligned} F_{\text{imp}} &= -\frac{1}{\beta} \ln Z_{\text{imp}} = -\frac{1}{\beta} \sum_{i\omega} \ln [-i\omega + h - i\pi\Gamma \cdot \text{sgn}(\omega)] e^{i\omega 0^+} \\ &= -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} f(\omega) \ln [-\omega + h + i\pi\Gamma] e^{\omega 0^+} + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} f(\omega) \ln [-\omega + h - i\pi\Gamma] e^{\omega 0^+}, \end{aligned} \quad (\text{E55})$$

where we have added the factor $e^{i\omega 0^+}$ for convergence. In the second line, the 1st (2nd) term is deformed from the contour in the lower (upper) half of the complex plane that generates the Matsubara summation over negative (positive) $i\omega$, respectively. $f(\omega) = 1/(e^{\frac{\omega}{T}} + 1)$ is the Fermi-Dirac function. Also, we need to specify the branches of the $\ln$ and arccot functions. To do this, we consider the limit $\Gamma \rightarrow 0^+$, where

$$F_{\text{imp}} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} f(\omega) \ln \left[\frac{\omega - h + i0^+}{\omega - h - i0^+} \right] = -\int_h^{\infty} d\omega f(\omega) = -T \ln[1 + e^{-h/T}] \quad (\text{E56})$$

In the second equality, we have specified $\ln(\omega - h + i0^+) = -i2\pi \cdot \theta(\omega - h) - i\pi\theta(h - \omega)$, $\ln(\omega - h - i0^+) = -i\pi\theta(h - \omega)$. In the third equality, we have exploited

$$f(\omega) = -T\partial_\omega [\ln(1 + e^{-\omega/T})] \quad (\text{E57})$$

With the current choice of branch cut, Eq. (E56) recovers the partition function of a standard two-level system with energies 0 and h , $Z = e^{-F_{\text{imp}}/T} = 1 + e^{-h/T}$.

Impurity entropy S_{imp} —At $\Gamma = 0$, with Eq. (E56), it can then be computed that

$$S_{\text{imp}} = -\frac{\partial F_{\text{imp}}}{\partial T} = \ln[1 + e^{-h/T}] + \frac{h}{T} \frac{1}{e^{h/T} + 1} = \ln[e^{h/2T} + e^{-h/2T}] - \frac{h}{2T} \tanh \frac{h}{2T} \quad (\text{E58})$$

If $\frac{h}{T} \rightarrow \infty$, $S_{\text{imp}} = 0$; if $\frac{h}{T} \rightarrow 0$, $S_{\text{imp}} = \ln 2$. At $\frac{h}{T} \gtrsim 1$, S_{imp} vanishes exponentially.

At finite Γ , based on Eq. (E57), integral-by-part for Eq. (E55) gives

$$\begin{aligned} F_{\text{imp}} &= T \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \ln \left(1 + e^{-\frac{\omega}{T}} \right) \left(\frac{-1}{\omega - h - i\pi\Gamma} + \frac{1}{\omega - h + i\pi\Gamma} \right) e^{\omega 0^+} \\ &= -T \int_{-\infty}^{\infty} d\omega \ln \left(1 + e^{-\frac{\omega}{T}} \right) \frac{1}{\pi} \frac{\pi\Gamma}{(\omega - h)^2 + (\pi\Gamma)^2} e^{\omega 0^+}, \end{aligned} \quad (\text{E59})$$

By comparing Eq. (E59) and Eq. (E56), one finds that, the free-energy at finite Γ and fixed h is equivalent to an “average” over an ensemble of systems with $\Gamma = 0$, but with some “error” in h of the order $\pi\Gamma$. Systems in such an ensemble appear with probabilities $\delta_{\pi\Gamma}(\omega - h) = \frac{1}{\pi} \frac{\pi\Gamma}{(\omega - h)^2 + (\pi\Gamma)^2}$. Accordingly, S_{imp} will follow the same “ensemble average”.

Therefore, at $h = 0$, if $\pi\Gamma \gg T$, only a small fraction ($\sim \frac{T}{\pi\Gamma}$) of systems in the ensemble has $S_{\text{imp}} = \ln 2$, while the remaining systems have $S_{\text{imp}} = 0$, hence the ensemble average will asymptote to 0. On the other hand, if $\pi\Gamma \ll T$, almost all systems in the ensemble will have $S_{\text{imp}} = \ln 2$, hence the ensemble average will asymptotes to $\ln 2$.

Static longitudinal susceptibility $\chi_z(0)$ —We also start with the $\Gamma = 0$ case. The magnetization can be computed as $M = \frac{1}{2}\langle\Lambda_z\rangle = \langle f_v^\dagger f_v \rangle - \frac{1}{2} = \frac{\partial F_{\text{imp}}}{\partial h} - \frac{1}{2} = \frac{1}{e^{h/T} + 1} - \frac{1}{2}$. At $h = 0$, we get a background value $M = 0$. The longitudinal susceptibility is given by

$$\chi_z(0) = -\frac{\partial M}{\partial h} = \frac{1}{T} \frac{1}{e^{h/T} + e^{-h/T} + 2} \quad (\text{E60})$$

Without h (and since without Γ), it scales as $1/T$, the Curie's law. When h is larger than T , $\chi_z(0)$ gets frozen to 0 exponentially. At finite Γ , since $\partial_\omega \delta_{\pi\Gamma}(\omega - h) = -\partial_h \delta_{\pi\Gamma}(\omega - h)$,

$$\begin{aligned} \chi_z(0) &= -\frac{\partial^2 F}{\partial h^2} = -T \int_{-\infty}^{\infty} d\omega \ln(1 + e^{-\beta\omega}) (-\partial_h^2) \frac{1}{\pi} \frac{\pi\Gamma}{(\omega - h)^2 + (\pi\Gamma)^2} \\ &= -T \int_{-\infty}^{\infty} d\omega \ln(1 + e^{-\beta\omega}) (-\partial_\omega^2) \frac{1}{\pi} \frac{\pi\Gamma}{(\omega - h)^2 + (\pi\Gamma)^2} \\ &= \int_{-\infty}^{\infty} d\omega \frac{1}{T} \frac{1}{e^{\omega/T} + e^{-\omega/T} + 2} \frac{1}{\pi} \frac{\pi\Gamma}{(\omega - h)^2 + (\pi\Gamma)^2} \end{aligned} \quad (\text{E61})$$

which is given by the “ensemble average” likewise. At $h = 0$, if $\pi\Gamma \gg T$, then only a fraction of $\frac{T}{\pi\Gamma}$ systems in the ensemble exhibits unfrozen susceptibility $\sim \frac{1}{T}$, hence the total susceptibility averages to $\chi^z(0) \sim \frac{1}{\pi\Gamma}$, which is the typical behavior of FL at low temperature. If $T \gg \pi\Gamma$, on the other hand, the whole ensemble exhibits Curies' law, hence $\chi_z(0) \sim \frac{1}{T}$.

4. Impurity correlation functions

In this section, we compute correlation functions (dynamic susceptibilities). Finite-size terms of $\mathcal{O}(L^{-1})$ are still omitted in the thermodynamic limit. It is useful to work out the correlation functions of the pseudo-fermions first, as physical correlation functions will eventually be expressed in terms of them. From Eq. (E52) (see Sec. E3), setting $h = 0$, it is direct to read off the Green's function for f_v fermions as

$$\mathcal{G}_f(i\omega) = \frac{1}{i\omega + i \cdot \text{sgn}(\omega) \cdot \pi\Gamma} \quad (\text{E62})$$

We use $\mathcal{G}_f$ for the Green's function of the pseudo-fermions f_v , in order to distinguish from the Green's function of the physical f electron. Fourier Eq. (E62) to the imaginary time axis τ , we obtain

$$\begin{aligned} \mathcal{G}_f(\tau) &= \frac{1}{\beta} \sum_{i\omega} G_f(i\omega) e^{-i\omega\tau} \stackrel{T \rightarrow 0^+}{=} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathcal{G}_f(i\omega) e^{-i\omega\tau} = - \int_0^{\infty} \frac{d\omega}{\pi} \frac{\sin(\omega\tau)}{\omega + \pi\Gamma} \\ &= - \int_{\pi\Gamma\tau}^{\infty} \frac{dx}{\pi} \frac{\sin(x) \cos(\pi\Gamma\tau) - \cos(x) \sin(\pi\Gamma\tau)}{x} \\ &= - \left(\frac{1}{2} - \frac{\text{Si}(\pi\Gamma\tau)}{\pi} \right) \cos(\pi\Gamma\tau) - \frac{\text{Ci}(\pi\Gamma\tau)}{\pi} \sin(\pi\Gamma\tau) = -\frac{1}{\Gamma\tau} + \mathcal{O}\left(\frac{1}{(\Gamma\tau)^2}\right) \quad \text{as } \Gamma\tau \gg 1 \end{aligned} \quad (\text{E63})$$

Here we have exploited

$$\begin{aligned} \text{Si}(z) &= \int_0^z dt \frac{\sin(t)}{t} = \frac{\pi}{2} - \frac{\cos(z)}{z} + \mathcal{O}\left(\frac{1}{z^2}\right) \quad \text{as } z \rightarrow \infty \\ \text{Ci}(z) &= - \int_z^{\infty} dt \frac{\cos(t)}{t} = \frac{\sin(z)}{z} + \mathcal{O}\left(\frac{1}{z^2}\right) \quad \text{as } z \rightarrow \infty. \end{aligned} \quad (\text{E64})$$

Now we compute the longitudinal correlation function

$$\chi_z(\tau) = -\langle T_\tau e^{\tau H} \cdot \Lambda_z \cdot e^{-\tau H} \cdot \Lambda_z \rangle_0 = -\langle T_\tau e^{\tau \hat{H}_{\text{PK}}} \cdot (2f_v^\dagger f_v - 1) \cdot e^{-\tau \hat{H}_{\text{PK}}} \cdot (2f_v^\dagger f_v - 1) \rangle_{\hat{0}} \quad (\text{E65})$$

Here, states $|G\rangle$ in the $\hat{0}$ gauge are transformed to 0 gauge according to $|G\rangle = U^\dagger U_2^\dagger |\hat{G}\rangle$. Recall that $U_2 = e^{i\frac{\pi}{4} N_v \Lambda_z}$, and $U = e^{i\frac{1}{2} \Lambda_z \phi_v(0)}$ at $\rho_z^* = \frac{1}{4}$. In terms of the pseudo-fermions, $2f_v^\dagger f_v - 1$ measures the density fluctuation of f_v fermions. As they are non-interacting,

$$\chi_z(\tau) = -\mathcal{G}_f(\tau) \mathcal{G}_f(-\tau) = -\frac{1}{(\Gamma\tau)^2} + \mathcal{O}\left(\frac{1}{(\Gamma\tau)^3}\right) \quad \text{at } \Gamma\tau \gg 1 \quad (\text{E66})$$

By comparing to Sec. C2, we conclude that the scaling in the imaginary time domain as $\frac{1}{\tau^2}$ will imply that the dynamic susceptibility to scale as $\text{Im}\chi_z^R(\omega) \sim -\frac{\omega}{\Gamma^2}$, which is the Fermi liquid behavior.

Let us also evaluate the transverse correlation function,

$$\begin{aligned}
\chi_x(\tau) &= -\langle T_\tau e^{\tau H} \cdot \Lambda_+ \cdot e^{-\tau H} \cdot \Lambda_- \rangle_0 = -\left\langle T_\tau e^{\tau \bar{H}} \cdot e^{i\phi_v(0)} \Lambda_+ \cdot e^{-\tau \bar{H}} \cdot \Lambda_- e^{-i\phi_v(0)} \right\rangle_{\bar{0}} \\
&= -\left\langle T_\tau e^{\tau \bar{H}} \cdot F_v^\dagger e^{i\phi_v(0)} \Lambda_+ \cdot e^{-\tau \bar{H}} \cdot \Lambda_- F_v e^{-i\phi_v(0)} \right\rangle_{\bar{0}} \\
&= -\left\langle T_\tau e^{\tau \hat{H}_{\text{PK}}} \cdot \left(F_v^\dagger e^{i\frac{\pi}{2}\Lambda_z} \right) e^{i\phi_v(0)} \left(\Lambda_+ e^{i\frac{\pi}{2}N_v} \right) \cdot e^{-\tau \hat{H}_{\text{PK}}} \cdot \left(\Lambda_- e^{-i\frac{\pi}{2}N_v} \right) \left(F_v e^{-i\frac{\pi}{2}\Lambda_z} \right) e^{-i\phi_v(0)} \right\rangle_{\hat{0}} \\
&= -(2\pi x_c) \left\langle T_\tau e^{\tau \hat{H}_{\text{PK}}} \cdot \psi_v^\dagger(0) f_v^\dagger \cdot e^{-\tau \hat{H}_{\text{PK}}} \cdot f_v \psi_v(0) \right\rangle_{\hat{0}}
\end{aligned} \tag{E67}$$

In the second line we inserted an identity $1 = F_v^\dagger F_v$, and used the fact that F_v commutes with $\bar{H}$. In the third line, we have carried out the gauge transformation U_2 , and used that $U_2 F_v U_2^\dagger = F_v e^{-i\frac{\pi}{2}\Lambda_z}$, and $U_2 \Lambda_\pm U_2^\dagger = \Lambda_\pm e^{i\frac{\pi}{2}N_v}$. In the fourth line, we have exploited the definition Eq. (E4), $f_v^\dagger = e^{i\frac{\pi}{2}N_v} \Lambda_+ e^{-i\frac{\pi}{2}\Lambda_z} = e^{i\frac{\pi}{2}N_v} e^{i\frac{\pi}{2}\Lambda_z} \Lambda_+$, because $e^{i\frac{\pi}{2}\Lambda_z} = i \cdot \Lambda_z$, which anti-commutes with $\Lambda_\pm$. At this stage, we find that the transverse susceptibility is given by a pairing correlation function of the pseudo-fermions. We do not explicitly evaluate the expression, but only remark that, at $\omega \ll \mathcal{O}(\Gamma)$, the system is nothing but a non-interacting Fermi liquid with π phase shift. Consequently, the pairing correlation function will also scale as $\frac{1}{\tau^2}$, implying that $\text{Im}\chi_x^R(\omega) \sim \omega$.

F. RG analysis in the singlet regime

Calculations in this section parallel with that in Sec. D.

1. Coulomb gas analog

The Hamiltonian that includes a potential phase transition to the LS phase is given by $\bar{H} = \bar{H}_0 + \bar{H}_x$, derived in Sec. B 4 (see Eqs. (B45) and (B46)). It has gone through a gauge transformation $U = e^{i\sqrt{2}\rho_z\Lambda_z(\varphi_\uparrow(0)+\varphi_\downarrow(0))}$. We re-write them here in a more convenient form,

$$\bar{H}_0 = \sum_{s=\uparrow,\downarrow} \int \frac{dx}{4\pi} : (\partial_x \varphi_s)^2 : + \frac{\varepsilon_D}{x_c} \cdot \mathbb{P}_D \quad (\text{F1})$$

$$\bar{H}_x = \frac{\zeta_x}{x_c} \sum_{\nu=\pm} \Theta_\nu \cdot \sum_{s=\uparrow,\downarrow} F_s^{(-\nu)} \cdot e^{-i\nu \vec{\xi}_s \cdot \vec{\varphi}} \quad (\text{F2})$$

Here, we have defined $F_s^{(-)} = F_s = F_{-s}^\dagger F_{+s}$, $F_s^{(+)} = F_s^\dagger$, which are composite Klein factors carrying the bath $U(1)_\nu$ charges per spin sector $s = \uparrow, \downarrow$. We have introduced the notations $\vec{\varphi} = (\varphi_\uparrow, \varphi_\downarrow)$ and

$$\vec{\xi}_\uparrow = (\sqrt{2}, 0) - \sqrt{2}(\rho_z, \rho_z) \quad \vec{\xi}_\downarrow = (0, \sqrt{2}) - \sqrt{2}(\rho_z, \rho_z). \quad (\text{F3})$$

Basically, ν keeps track of how the $U(1)_\nu$ charge is exchanged between the impurity and bath, which is conserved in total, while $s = \uparrow, \downarrow$ indicates which spin sector (channel) of the bath has participated in the exchange. We also define $\frac{\xi^2}{2} = \frac{\nu^2 \xi_s^2}{2} = 2\rho_z^2 - 2\rho_z + 1$, which is the scaling dimension of the vertex operators. For $0 < \rho_z < \frac{1}{2}$, $1 > \frac{\xi^2}{2} > \frac{1}{2}$ (monotonically) respectively. Also, note that $\vec{\xi}_\uparrow$ and $\vec{\xi}_\downarrow$ are linearly independent for all ρ_z .

We remark again the impurity operators are

$$\Lambda_z = |2\rangle\langle 2| - |\bar{2}\rangle\langle \bar{2}|, \quad \Theta_+ = |2\rangle\langle 0| + |0\rangle\langle \bar{2}|, \quad \Theta_- = |0\rangle\langle 2| + |\bar{2}\rangle\langle 0|, \quad (\text{F4})$$

where $|2\rangle, |\bar{2}\rangle$ form the doublet D and $|0\rangle = |S\rangle$ is the singlet. We take $\varepsilon_D > 0$ to illustrate the phase transition to LS.

The model is solvable if $\zeta_x = 0$, and we denote the partition function at $\zeta_x = 0$ as Z_0 . The total partition function Z at finite ζ_x is given by a perturbative expansion,

$$\delta Z = \frac{Z}{Z_0} = e^{-\delta F/T} = \left\langle T_\tau \exp \left(- \int_{-\frac{1}{2T}}^{\frac{1}{2T}} \bar{H}_x(\tau) \right) \right\rangle_{\bar{0}} = \sum_{n=0}^{\infty} \delta Z_{2n} \quad (\text{F5})$$

where $\delta Z_{2n} = \int_{(-\frac{1}{2T}, \frac{1}{2T})}^{>0} d^{2n}\tau \left\langle \bar{H}_x(\tau_{2n}) \bar{H}_x(\tau_{2n-1}) \cdots \bar{H}_x(\tau_2) \bar{H}_x(\tau_1) \right\rangle_{\bar{0}}$

Here δF is the additive correction to the free energy, T is the temperature, the subscript $\bar{0}$ represents average with respect to the equilibrium ensemble of $\bar{H}_0$. Such an ensemble differs from the equilibrium ensemble of free bosons/fermions only by a gauge transformation U . In the zero-temperature limit, $T \ll \frac{\varepsilon_D}{x_c}$, only the S manifold enters the ensemble average $\langle \cdots \rangle_{\bar{0}}$, T_τ is the time-ordering operator, hence $\int_{(-\frac{1}{2T}, \frac{1}{2T})}^{>0} d^{2n}\tau$ (defined in Eq. (D7)) represents the integral in the domain $\tau_{2n} > \tau_{2n-1} \cdots > \tau_2 > \tau_1$.

$$\bar{H}_x(\tau) = e^{\tau \bar{H}_0} \bar{H}_x e^{-\tau \bar{H}_0} = \frac{\zeta_x}{x_c} \sum_{\nu=\pm} \Theta_\nu(\tau) \sum_{s=\uparrow,\downarrow} F_s^{(-\nu)} \cdot e^{-i\nu \vec{\xi}_s \cdot \vec{\varphi}(\tau)} \quad (\text{F6})$$

writes the operators in the interacting picture. Crucially, there is no time-evolution for Klein factors, hence $F_s(\tau) = F_s$, while the impurity operators are evolved as

$$\Theta_+(\tau) = e^{\frac{\varepsilon_D}{x_c} \tau} \cdot |2\rangle\langle 0| + e^{-\frac{\varepsilon_D}{x_c} \tau} \cdot |0\rangle\langle \bar{2}|, \quad \Theta_-(\tau) = e^{-\frac{\varepsilon_D}{x_c} \tau} \cdot |0\rangle\langle 2| + e^{\frac{\varepsilon_D}{x_c} \tau} \cdot |\bar{2}\rangle\langle 0|. \quad (\text{F7})$$

We have omitted the spatial argument of φ_s for simplicity as they always locate at $x = 0$ in this section.

Following the discussions in Sec. D 1, as in $\bar{H}_0$ the impurity and the bath are decoupled, the ensemble average $\bar{\cdot}$ can be factorized into an average over impurity operators and an average over the bath, as

$$\delta Z_{2n} = \frac{\zeta_x^{2n}}{x_c^{2n}} \int_{(-\frac{1}{2T}, \frac{1}{2T})}^{>0} d^{2n}\tau \sum_{\{\nu\}} \left\langle \Theta_{\nu_{2n}}(\tau_{2n}) \cdots \Theta_{\nu_2}(\tau_2) \Theta_{\nu_1}(\tau_1) \right\rangle_{\bar{0}} \quad (F8)$$

$$\times \sum_{\{s\}} \left\langle F_{s_{2n}}^{(\bar{\nu}_{2n})} \cdots F_{s_1}^{(\bar{\nu}_1)} \right\rangle_{\bar{0}} \left\langle e^{-i\nu_{2n}\vec{\xi}_{s_{2n}} \cdot \vec{\varphi}(\tau_{2n})} \cdots e^{-i\nu_1\vec{\xi}_{s_1} \cdot \vec{\varphi}(\tau_1)} \right\rangle_{\bar{0}},$$

Here, $\sum_{\{\nu\}}$ and $\sum_{\{s\}}$ indicates the summation over all $\nu_i = \pm$ and $s_i = \uparrow, \downarrow$, respectively. We now analyze the general structure of all non-vanishing terms in the summation $\sum_{\{\nu\}} \sum_{\{s\}}$.

For the impurity average, as $\bar{0}$ only contains the $|0\rangle$ state in the zero-temperature limit, Θ_{ν_1} should only excite it to *either* $|2\rangle$ or $|\bar{2}\rangle$, while Θ_{ν_2} should then lower it back to $|0\rangle$. Therefore, there must be $\nu_2 = \bar{\nu}_1$, where ν_1 can be either $+$ or $-$. The same analysis can be recursively applied to any $\Theta_{\nu_{2k}} \Theta_{\nu_{2k-1}}$. Therefore, the non-vanishing terms in $\sum_{\{\nu\}}$ are given by all configurations of ν that satisfies $\nu_{2k} = \bar{\nu}_{2k-1} = +$ or $\nu_{2k} = \bar{\nu}_{2k-1} = -$. In total, there are 2^n different such configurations.

Since between $\tau_{2k} - \tau_{2k-1}$ the impurity always stays at the high-energy D manifold, it accumulates a factor $e^{-\frac{\varepsilon_D}{x_c}(\tau_{2k} - \tau_{2k-1})}$ according to Eq. (F7). The full impurity average value thus always equals to

$$\left\langle \Theta_{\nu_{2n}}(\tau_{2n}) \cdots \Theta_{\nu_1}(\tau_1) \right\rangle_{\bar{0}} = e^{-\frac{\varepsilon_D}{x_c} \sum_i^n (\tau_{2i} - \tau_{2i-1})} \quad \text{for all configurations } \{\nu\}. \quad (F9)$$

For each configuration of $\{\nu\}$, one can assign s_i to $i = 1, \dots, 2n$ independently, with the only requirement being that the bath valley charge per spin flavor (accumulated by $F_{\uparrow}$ and $F_{\downarrow}$, respectively) are both zero. In other words, this is equivalent to requiring the total bath charge is zero, $\sum_i \nu_i = 0$, which is already satisfied, and requiring that the “spin-contrasting” bath charge is also zero, $\sum_i \nu_i s_i = 0$. It is convenient to regard the quantities $\nu_i s_i$ as independent variables, and n out of $2n$ of them should be $+$, with the remaining ones being $-$. Thus, for a given configuration of $\{\nu\}$, there are $\binom{2n}{n}$ configurations of $\{s\}$.

It can be shown that $F_{\uparrow}$ commutes with $F_{\downarrow}$ and $F_{\downarrow}^{\dagger}$. Therefore, the product of Klein factors is trivially 1. The remaining average over the vertex operators are given by Eq. (A61),

$$\left\langle e^{-i\nu_{2n}\vec{\xi}_{s_{2n}} \cdot \vec{\varphi}(\tau_{2n})} \cdots e^{-i\nu_1\vec{\xi}_{s_1} \cdot \vec{\varphi}(\tau_1)} \right\rangle_{\bar{0}} = \exp \left(- \sum_{j>i} \nu_j \nu_i (\vec{\xi}_{s_j} \cdot \vec{\xi}_{s_i}) \ln \left(\frac{\pi T x_c}{\sin(\pi T(\tau_j - \tau_i) + \pi T x_c)} \right) \right). \quad (F10)$$

To sum up, we have

$$\delta Z_{2n} = \frac{\zeta_x^{2n}}{x_c^{2n}} \int_{(-\frac{1}{2T}, \frac{1}{2T})}^{>0} d^{2n}\tau e^{-\frac{\varepsilon_D}{x_c} \sum_i^n (\tau_{2i} - \tau_{2i-1})} \sum'_{\{\nu\}} \sum'_{\{s\}} \exp \left(- \sum_{j>i} \nu_j \nu_i (\vec{\xi}_{s_j} \cdot \vec{\xi}_{s_i}) \ln \left(\frac{\pi T x_c}{\sin(\pi T(\tau_j - \tau_i) + \pi T x_c)} \right) \right) \quad (F11)$$

where $\sum'_{\{\nu\}} \sum'_{\{s\}}$ only selects out the non-vanishing configurations.

As we did in Sec. D 1, we replace $\ln \left(\frac{\pi T x_c}{\sin(\pi T(\tau_j - \tau_i) + \pi T x_c)} \right)$ by $\ln \left(\frac{x_c}{\tau_j - \tau_i} \right)$ in the zero-temperature limit, and correspondingly change the integral range $\int_{(-\frac{1}{2T}, \frac{1}{2T})}^{>0} d^{2n}\tau$ to $\int_{(-\frac{1}{2T}, \frac{1}{2T})}^{>x_c} d^{2n}\tau$. The factor $e^{-\frac{\varepsilon_D}{x_c}(\tau_{2i} - \tau_{2i-1})}$ also changes to $e^{-\frac{\varepsilon_D}{x_c}(\tau_{2i} - \tau_{2i-1})} \cdot e^{\varepsilon_D}$. We then rewrite the partition function as

$$\delta Z_{2n} = \frac{\zeta_x^{2n}}{x_c^{2n}} e^{n \cdot \varepsilon_D} \int_{(-\frac{1}{2T}, \frac{1}{2T})}^{>x_c} d^{2n}\tau e^{-\frac{\varepsilon_D}{x_c} \sum_{i=1}^n (\tau_{2i} - \tau_{2i-1})} \sum'_{\{\nu\}} \sum'_{\{s\}} \exp \left(- \sum_{j>i} \nu_j \nu_i (\vec{\xi}_{s_j} \cdot \vec{\xi}_{s_i}) \ln \left(\frac{x_c}{\tau_j - \tau_i} \right) \right). \quad (F12)$$

The partition function above Eq. (F12) describes $2n$ particles on a line, interacting through two types of Coulomb forces: a 1D Coulomb potential proportional to $\frac{\varepsilon_D}{x_c} |\tau_{j'} - \tau_j|$, and a 2D logarithmic Coulomb potential proportional to $\ln \frac{x_c}{|\tau_{j'} - \tau_j|}$. The 1D Coulomb charge of the particles are given by $(-1)^j$, while the 2D Coulomb charge of the particles are given by a vector $\nu_j \vec{\xi}_{s_j}$. Whether the 2D Coulomb force is repulsive or attractive depends on the inner product between two “vector charges”. Below we explain this analog in detail.

First, $\frac{\varepsilon_D}{x_c}(\tau_{2i} - \tau_{2i-1}) = \frac{\varepsilon_D}{x_c} |\tau_{2i} - \tau_{2i-1}|$ (because we have sorted $\tau_{2i} > \tau_{2i-1}$) can be interpreted as a 1D Coulomb potential between two particles with distance $|\tau_{2i} - \tau_{2i-1}|$, because its derivative with respect to the distance, the electric field strength, will be constant. The two particles possess opposite 1D Coulomb charge, as the potential energy grows with increasing distance

$|\tau_{2i} - \tau_{2i-1}|$. More generically, we can assign the particle at τ_j with a 1D Coulomb charge $(-1)^j$, and the total energy will simplify to

$$-\sum_{j' > j} (-1)^{j'-j} (\tau_{j'} - \tau_j) = \sum_{i=1}^n (\tau_{2i} - \tau_{2i-1}) \quad (\text{F13})$$

The proof is simple. For a particle at τ_{2i-1} , all the particles τ_j to its right ($2-i > j$) possess a vanishing total charge. As the 1D Coulomb force do not decay, the vanishing total charge also implies an exactly vanishing total Coulomb force. On the other hand, all the particles $\tau_{j'}$ to its left ($j' > 2i-1$) possess a +1 total charge, hence attracting τ_{2i-1} to its left. Similarly, one can show that τ_{2i} is attracted to its right. The net effect will thus be equivalent to only counting the interaction between τ_{2i} and τ_{2i-1} .

We also remark that, since the two particles have a minimal distance x_c , the minimal energy cost of the 1D Coulomb interactions correspond to a factor of $e^{-n\varepsilon_D}$ in the partition function, which will be compensated by the pre-factor $e^{n\varepsilon_D}$. Therefore, ζ_x still represents the fugacity.

For the 2D Coulomb force, it takes a similar form with Sec. D, with the only difference being that the 2D Coulomb charge behaves as a vector $\nu_j \vec{\xi}_{sj}$, and the Coulomb potential between a particle pair is proportional to the inner product of the “vector charges”.

To gain some insights into the perturbation theory, let us calculate the lowest order correction δZ_2 ,

$$\delta Z_2 = 4 \frac{\zeta_x^2}{x_c^2} e^{\varepsilon_D} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 e^{-\frac{\varepsilon_D}{x_c}(\tau_2 - \tau_1)} \left(\frac{x_c}{\tau_2 - \tau_1} \right)^{\xi^2}. \quad (\text{F14})$$

where $\xi^2 = 2 - 4\rho_z + 4\rho_z^2$. The factor $4 = 2 \times 2$ originates from the summation $\sum'_{\{\nu\}} \sum'_{\{s\}}$, where $\nu_1 = \pm$ and $s_1 = \uparrow, \downarrow$ in total contribute four equal terms. Since $e^{\varepsilon_D - \frac{\varepsilon_D}{x_c}(\tau_2 - \tau_1)} \leq 1$ for $\varepsilon_D \geq 0$, any finite ε_D will suppress the partition function correction from ζ_x , and will guarantee the integral over $d\tau_1$ to be convergent. Integrating over $d\tau_1$ yields $x_c E_{2-4\rho_z+4\rho_z^2}(\varepsilon_D)$, where $E_n(x) = \int_1^\infty dt e^{-xt} t^{-n}$ is exponential integral function. Therefore, $\delta Z_2 = 4 \frac{\zeta_x^2}{T x_c} \cdot e^{\varepsilon_D} \cdot E_{2-4\rho_z+4\rho_z^2}(\varepsilon_D)$, hence the $\mathcal{O}(\zeta_x^2)$ correction to the ground state energy is

$$\begin{aligned} \delta E_2 &= -T \cdot \delta Z_2 = -4 \frac{\zeta_x^2}{x_c} e^{\varepsilon_D} \cdot E_{2-4\rho_z+4\rho_z^2}(\varepsilon_D) \\ &= -4 \frac{\zeta_x^2}{x_c} e^{\varepsilon_D} \left(\frac{1}{(1-2\rho_z)^2} + \varepsilon_D^{(1-2\rho_z)^2} \cdot \Gamma(-(1-2\rho_z)^2) + \frac{\varepsilon_D}{4\rho_z(1-\rho_z)} + \mathcal{O}(\varepsilon_D^2) \right), \end{aligned} \quad (\text{F15})$$

where $\Gamma(x)$ is the Γ -function.

2. Flow equations

To obtain the RG flow, we use a “coarser” coordinate by rewriting $\tau = b\tau'$, where $b = e^{d\ell} > 1$, and then relabeling τ' as τ . Then the partition function in Eq. (F12) becomes

$$\delta Z_{2n} = \frac{\zeta_x^{2n}}{x_c^{2n}} b^{2n} b^{-2n(1-2\rho_z+2\rho_z^2)} e^{n\varepsilon_D} \int_{(-\frac{1}{2T}, \frac{1}{2T})}^{>x_c b^{-1}} d^{2n}\tau e^{-b\frac{\varepsilon_D}{x_c} \sum_{i=1}^n (\tau_{2i} - \tau_{2i-1})} \sum'_{\{\nu\}} \sum'_{\{s\}} \prod_{j>i} \left(\frac{x_c}{\tau_j - \tau_i} \right)^{-\nu_j \nu_i \vec{\xi}_{sj} \cdot \vec{\xi}_{si}}. \quad (\text{F16})$$

The factor b^{2n} originates from rescaling the integral measure, and $b^{\sum_{j>i} \nu_j \nu_i \vec{\xi}_{sj} \cdot \vec{\xi}_{si}} = b^{-2n(1-2\rho_z+2\rho_z^2)}$ originates from rescaling the 2D Coulomb factors. To be more concrete, since for all configuration $\{\nu\}, \{s\}$, there is $\sum_{i=1}^{2n} \nu_i \vec{\xi}_{si} = 0$, we obtain

$$\sum_{j>i} \nu_j \nu_i \vec{\xi}_{sj} \cdot \vec{\xi}_{si} = \frac{1}{2} \sum_{j,i} (\nu_j \vec{\xi}_{sj}) \cdot (\nu_i \vec{\xi}_{si}) - \frac{1}{2} \sum_i \nu_i^2 \vec{\xi}_i^2 = -2n(1-2\rho_z+2\rho_z^2) \quad (\text{F17})$$

For the 1D Coulomb, the rescaled effective coupling reads $\varepsilon'_D = \varepsilon_D e^{d\ell}$, while the rescaled fugacity satisfies $\zeta'_x \cdot e^{\frac{\varepsilon'_D}{2}} = \zeta_x \cdot b^{1-(1-2\rho_z+2\rho_z^2)} e^{\frac{\varepsilon_D}{2}}$. Therefore, $\zeta'_x = \zeta_x \cdot e^{d\ell(2\rho_z-2\rho_z^2)} \cdot e^{\frac{1}{2}(\varepsilon_D - e^{d\ell}\varepsilon_D)} = \zeta_x \cdot e^{d\ell(2\rho_z-2\rho_z^2-\frac{\varepsilon_D}{2})}$. These relations imply the tree-level RG flow equations

$$\frac{d\zeta_x}{d\ell} = \left(2\rho_z - 2\rho_z^2 - \frac{1}{2}\varepsilon_D \right) \zeta_x, \quad \frac{d\varepsilon_D}{d\ell} = \varepsilon_D. \quad (\text{F18})$$

To derive the higher-order correction to the flow equations, we need to integrate out “high-energy” configurations where distances between adjacent particles are smaller than x_c . Following the discussions around Eq. (D18) in Sec. D, we need to calculate $\delta Z_{2,1}$ and $\delta Z_{4,1}$. $\delta Z_{2,1}$ is δZ_2 where $x_c b^{-1} < \tau_2 - \tau_1 < x_c$. Since the integral over τ_2 is proportional to $d\ell$ and only $\mathcal{O}(d\ell)$ terms are of interest, we can neglect the b factors elsewhere. It is straightforward to obtain

$$\delta Z_{2,1} = 4 \frac{\zeta_x^2}{T x_c} \cdot d\ell + \mathcal{O}(d\ell^2). \quad (\text{F19})$$

$\delta Z_{4,1}$ consists of three terms, $\delta Z_{4,1} = \sum_{i=1}^3 \delta Z_{4,1}^{(i+1,i)}$, where $\delta Z_{4,1}^{(i+1,i)}$ has a molecule formed by τ_{i+1} and τ_i . The first term is

$$\delta Z_{4,1}^{(2,1)} = \frac{\zeta_x^4}{x_c^4} e^{2\varepsilon_D} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_4 \int_{-\frac{1}{2T}}^{\tau_4 - x_c} d\tau_3 \int_{-\frac{1}{2T}}^{\tau_3 - x_c} d\tau_2 \int_{\tau_2 - x_c}^{\tau_2 - x_c/b} d\tau_1 e^{-\frac{\varepsilon_D}{x_c}(\tau_4 - \tau_3 + \tau_2 - \tau_1)} \sum_{\{\nu\}}' \sum_{\{s\}}' \prod_{j>i} \left(\frac{x_c}{\tau_j - \tau_i} \right)^{-\nu_j \nu_i \vec{\xi}_{s_j} \cdot \vec{\xi}_{s_i}}. \quad (\text{F20})$$

A complication comes from the summation $\sum_{\{\nu\}}' \sum_{\{s\}}'$. Unlike the case in doublet regime (Sec. D), the molecule at (τ_2, τ_1) is not necessarily charge neutral, i.e., $\nu_2 \vec{\xi}_2 + \nu_1 \vec{\xi}_1 = 0$.

We now argue that, for generic $\delta Z_{4,1}^{(i+1,i)}$, only the contribution from *neutral* molecule (or dipole) at (τ_{i+1}, τ_i) is relevant. We introduce the vector charge $\vec{\zeta}_i = \nu_i \vec{\xi}_{s_i}$ for the particle at τ_i , and the total vector charge $\vec{\zeta}_0 = \vec{\zeta}_{i+1} + \vec{\zeta}_i$ for the molecule to be integrated out. Since the total charge of the $2n+2$ particles vanishes, there must be $\sum_{j \neq i, i+1} \vec{\zeta}_j = -\vec{\zeta}_0$. Then a typical value of the integrand, where distances between remaining particles are typically $\sim T$, is $(x_c T)^{n(2-4\rho_z+4\rho_z^2)+\frac{1}{2}\vec{\zeta}_0^2}$. Thus, terms with $\vec{\zeta}_0 \neq 0$ are typically smaller by a factor of $\mathcal{O}((x_c T)^{\frac{1}{2}\vec{\zeta}_0^2})$. We will only keep neutral molecule in the following calculations.

Given $\nu_2 \vec{\xi}_{s_2} + \nu_1 \vec{\xi}_{s_1} = 0$ and $\nu_2 = -\nu_1$, the remaining two particles in $\delta Z_{4,1}^{(2,1)}$ at τ_4 and τ_3 must carry $\nu_4 = -\nu_3$ and $s_4 = s_3$, as if they are variables for a two-particle partition function. With $\tau_2 - \tau_1 = x_c + \mathcal{O}(d\ell)$, the factor $\prod_{j>i} \left(\frac{x_c}{\tau_j - \tau_i} \right)^{-\nu_j \nu_i \vec{\xi}_{s_j} \cdot \vec{\xi}_{s_i}}$ becomes

$$\exp \left(\nu_4 \nu_3 \vec{\xi}_4 \cdot \vec{\xi}_3 \ln \left(\frac{\tau_4 - \tau_3}{x_c} \right) - \nu_4 \nu_1 \vec{\xi}_4 \cdot \vec{\xi}_1 \ln \left(\frac{\tau_4 - \tau_2}{\tau_4 - \tau_2 + x_c} \right) + \nu_3 \nu_1 \vec{\xi}_3 \cdot \vec{\xi}_1 \ln \left(\frac{\tau_3 - \tau_2 + x_c}{\tau_3 - \tau_2} \right) \right), \quad (\text{F21})$$

and the factor $e^{-\frac{\varepsilon_D}{x_c}(\tau_4 - \tau_3 + \tau_2 - \tau_1)}$ becomes

$$e^{-\frac{\varepsilon_D}{x_c}(\tau_4 - \tau_3)} \cdot e^{-\varepsilon_D}. \quad (\text{F22})$$

We relabel $i = 3, 4$ as $i = 1, 2$, respectively, and relabel the original $\nu_1 = -\nu_2$ as ν' , and the original $s_1 = s_2$ as s' . Also, relabel $\tau_2 = \tau' + \frac{1}{2}s$, where $x_c b^{-1} < s < x_c$. These primed variables will be integrated out as virtual processes. Following the calculations around Eq. (D21), we obtain

$$\begin{aligned} \delta Z_{4,1}^{(2,1)} &= \frac{\zeta_x^2}{x_c^2} e^{2\varepsilon_D} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 \sum_{\{\nu_2, \nu_1\}}' \sum_{\{s_2, s_1\}}' e^{-\frac{\varepsilon_D}{x_c}(\tau_2 - \tau_1)} \left(\frac{x_c}{\tau_2 - \tau_1} \right)^{-\nu_2 \nu_1 \vec{\xi}_{s_2} \cdot \vec{\xi}_{s_1}} \\ &\quad \times e^{-\varepsilon_D} \zeta_x^2 d\ell \sum_{\nu'=\pm} \sum_{s'=\uparrow\downarrow} \int_{-\frac{1}{2T}}^{\tau_1 - \frac{3}{2}x_c} d\tau' \left(\frac{1}{x_c} - \frac{\nu_2 \nu' \vec{\xi}_2 \cdot \vec{\xi}'}{\tau_2 - \tau'} + \frac{\nu_1 \nu' \vec{\xi}_1 \cdot \vec{\xi}'}{\tau_1 - \tau'} + \mathcal{O}(x_c) \right), \end{aligned} \quad (\text{F23})$$

In terms of the Coulomb gas analog, the second and third terms in the last row describe the interaction between a (virtual) 2D Coulomb dipole and the remaining particles. Importantly, there is $\sum_{\nu'=\pm} \sum_{s'=\uparrow\downarrow} \nu' \vec{\xi}_{s'} = 0$, namely, this dipole does not have a definite orientation, as opposed to the dipole in the pair-Kondo model (see Sec. D). Therefore, summing over all the possible dipole configurations will average out, and the second and third terms will vanish. Consequently, the 2D Coulomb interaction between the remaining particles will not be screened, and ρ_z will remain invariant. Integrating the non-vanishing terms over $d\tau'$ then produces

$$\delta Z_{4,1}^{(2,1)} = \frac{\zeta_x^2}{x_c^2} e^{2\varepsilon_D} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 \sum_{\{\nu\}}' \sum_{\{s\}}' e^{-\frac{\varepsilon_D}{x_c}(\tau_2 - \tau_1)} \left(\frac{x_c}{\tau_2 - \tau_1} \right)^{-\nu_2 \nu_1 \vec{\xi}_{s_2} \cdot \vec{\xi}_{s_1}} \cdot e^{-\varepsilon_D} \zeta_x^2 d\ell \cdot \frac{4}{x_c} \left(\frac{1}{2T} + \tau_1 \right). \quad (\text{F24})$$

Following the calculations around Eq. (D23), we also obtain

$$\delta Z_{4,1}^{(3,2)} = \frac{\zeta_x^2}{x_c^2} e^{2\varepsilon_D} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2 - x_c} d\tau_1 \sum_{\{\nu\}}' \sum_{\{s\}}' e^{-\frac{\varepsilon_D}{x_c}(\tau_2 - \tau_1)} \left(\frac{x_c}{\tau_2 - \tau_1} \right)^{-\nu_2 \nu_1 \vec{\xi}_{s_2} \cdot \vec{\xi}_{s_1}} \cdot e^{\varepsilon_D} \zeta_x^2 d\ell \cdot \frac{4}{x_c} (\tau_2 - \tau_1), \quad (\text{F25})$$

The major difference of $\delta Z_{4,1}^{(3,2)}$ from $\delta Z_{4,1}^{(2,1)}$ is the second e^{ε_D} factor, which comes from $e^{\frac{\varepsilon_D}{x_c}(\tau_3-\tau_2)}$ with (τ_3, τ_2) being the integrated molecule before we relabel the variables. Following the calculations around Eq. (D24), we obtain

$$\delta Z_{4,1}^{(4,3)} = \frac{\zeta_x^2}{x_c^2} e^{2\varepsilon_D} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2-x_c} d\tau_1 \sum_{\{\nu\}}' \sum_{\{s\}}' e^{-\frac{\varepsilon_D}{x_c}(\tau_2-\tau_1)} \left(\frac{x_c}{\tau_2-\tau_1} \right)^{-\nu_2\nu_1\vec{\xi}_{s_2}\cdot\vec{\xi}_{s_1}} \cdot e^{-\varepsilon_D} \zeta_x^2 d\ell \cdot \frac{4}{x_c} \left(\frac{1}{2T} - \tau_2 \right), \quad (\text{F26})$$

where the factor $e^{-\varepsilon_D}$ comes from $e^{-\frac{\varepsilon_D}{x_c}(\tau_4-\tau_3)}$ with (τ_4, τ_3) being the integrated molecule. Adding up the three terms, we obtain

$$\delta Z_{4,1} = \frac{\zeta_x^2}{x_c^2} e^{\varepsilon_D} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2-x_c} d\tau_1 \sum_{\{\nu\}}' \sum_{\{s\}}' e^{-\frac{\varepsilon_D}{x_c}(\tau_2-\tau_1)} \left(\frac{x_c}{\tau_2-\tau_1} \right)^{-\nu_2\nu_1\vec{\xi}_{s_2}\cdot\vec{\xi}_{s_1}} d\ell \frac{4\zeta_x^2}{x_c} \left(\frac{1}{T} + (e^{2\varepsilon_D} - 1)(\tau_2 - \tau_1) \right). \quad (\text{F27})$$

According to Eq. (D18), the renormalized two-particle partition function is $\delta Z_2' = \delta Z_{2,0} + \delta Z_{4,1} - \delta Z_{2,1}\delta Z_{2,0}$, where $\delta Z_{2,0}$ is rescaled as explained after Eq. (F16) and $\delta Z_{2,1} = 4\frac{\zeta_x^2}{x_c^2}e^{-\varepsilon_D}$ is given in Eq. (F19). The $\frac{1}{T}$ term in $\delta Z_{4,1}$ is exactly canceled by $\delta Z_{2,1}\delta Z_{2,0}$. Thus, the higher-order correction to $\delta Z_2'$ (in addition to the tree-level contribution) is

$$\begin{aligned} & \delta Z_{4,1} - \delta Z_{2,1}\delta Z_{2,0} \\ &= \frac{\zeta_x^2}{x_c^2} e^{\varepsilon_D} \int_{-\frac{1}{2T}}^{\frac{1}{2T}} d\tau_2 \int_{-\frac{1}{2T}}^{\tau_2-x_c} d\tau_1 \sum_{\{\nu\}}' \sum_{\{s\}}' e^{-\frac{\varepsilon_D}{x_c}(\tau_2-\tau_1)} \left(\frac{x_c}{\tau_2-\tau_1} \right)^{-\nu_2\nu_1\vec{\xi}_{s_2}\cdot\vec{\xi}_{s_1}} d\ell \frac{4\zeta_x^2}{x_c} (e^{2\varepsilon_D} - 1)(\tau_2 - \tau_1). \end{aligned} \quad (\text{F28})$$

The term $d\ell \frac{4\zeta_x^2}{x_c} (e^{2\varepsilon_D} - 1)(\tau_2 - \tau_1)$ can be absorbed as a correction $-4(e^{2\varepsilon_D} - 1)\zeta_x^2 d\ell$ to ε_D . It describes how a virtual 1D Coulomb dipole screens the 1D Coulomb interaction. Added with the tree-level flows, the flow equations are

$$\frac{d\varepsilon_D}{d\ell} = \varepsilon_D - 4(e^{2\varepsilon_D} - 1)\zeta_x^2 + \mathcal{O}(\zeta_x^3), \quad (\text{F29})$$

$$\frac{d\zeta_x}{d\ell} = \left(2\rho_z - 2\rho_z^2 - \frac{1}{2}\varepsilon_D \right) \zeta_x + \mathcal{O}(\zeta_x^3). \quad (\text{F30})$$

We will omit the $\mathcal{O}(\zeta_x^3)$ terms. It is worth emphasizing that ρ_z remains invariant up to the second order of ζ_x .

3. Phase diagram and critical exponent

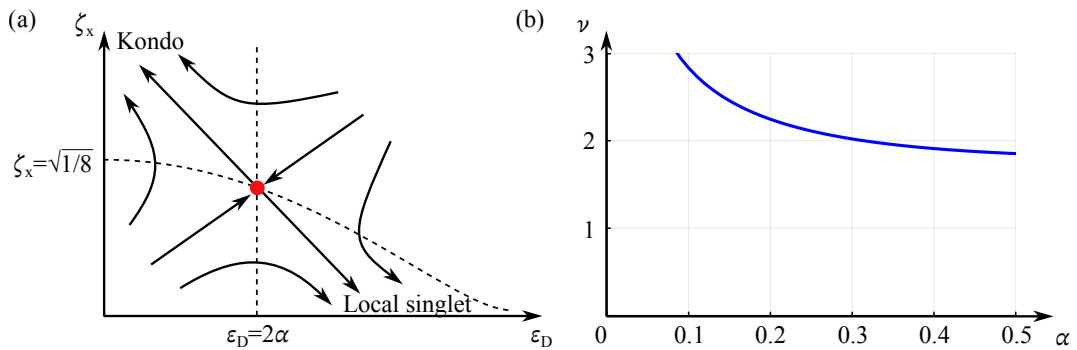


FIG. 9. RG flow in the singlet regime. (a) The vertical dashed line indicates $\varepsilon_D = 2\alpha$, and the dashed curve indicates $\zeta_x = \sqrt{\frac{\varepsilon_D}{4(e^{2\varepsilon_D} - 1)}}$. The red dot is the critical point. Here $\alpha = 2\rho_z - 2\rho_z^2$. (b) The critical exponent ν as a function of α .

For brevity, we define

$$\alpha = 2\rho_z - 2\rho_z^2 \in (0, \frac{1}{2}) \quad (\text{F31})$$

in this subsection. $\frac{d\zeta_x}{d\ell} = 0$ if $\varepsilon_D = 2\alpha$, and $\frac{d\varepsilon_D}{d\ell} = 0$ if $\zeta_x = \sqrt{\frac{\varepsilon_D}{4(e^{2\varepsilon_D}-1)}}$. We then derive the flow diagram shown in Fig. 9(a). The strong-coupling fixed point at $(\varepsilon_D, \zeta_x) = (0^+, \infty)$ represents the Kondo Fermi liquid, and the weak-coupling fixed point at $(\varepsilon_D, \zeta_x) = (\infty, 0^+)$ represents local-singlet Fermi liquid. They are separated by the critical point at $(\varepsilon_D, \zeta_x) = (2\alpha, \sqrt{\frac{\alpha}{2(e^{4\alpha}-1)}})$. To extract the critical exponent, we introduce $\delta\varepsilon_D = \varepsilon_D - 2\alpha$ and $\delta\zeta_x = \zeta_x - \sqrt{\frac{\alpha}{2(e^{4\alpha}-1)}}$, and expand the flow equations to linear order of $\delta\varepsilon_D$ and $\delta\zeta_x$:

$$\frac{d}{d\ell} \begin{pmatrix} \delta\varepsilon_D \\ \delta\zeta_x \end{pmatrix} = \begin{pmatrix} 1 - \frac{4e^{4\alpha}\alpha}{e^{4\alpha}-1} & -\frac{4\sqrt{2\alpha}}{\sqrt{e^{4\alpha}-1}} \\ -\frac{\sqrt{\frac{\alpha}{e^{4\alpha}-1}}}{2\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} \delta\varepsilon_D \\ \delta\zeta_x \end{pmatrix}. \quad (\text{F32})$$

The matrix on the right-hand side has a negative eigenvalue, which corresponds to an irrelevant parameter, and a positive eigenvalue, which corresponds to a relevant parameter t . The positive eigenvalue is

$$\frac{1}{\nu} = \frac{1}{2} + \frac{-4\alpha \cdot e^{4\alpha} + \sqrt{e^{8\alpha}(16\alpha^2 + 1) + 8\alpha - 2e^{4\alpha}(4\alpha + 1) + 1}}{2(e^{4\alpha} - 1)}. \quad (\text{F33})$$

The flow of the relevant parameter is $\frac{dt}{d\ell} = \frac{1}{\nu}t$. Without loss of generality, we take $t = 1$ as the strong-coupling fixed point. Then the RG time from a small positive t to the strong-coupling fixed point is $\ell = \nu \cdot \ln \frac{1}{t}$, suggesting a Kondo temperature

$$T_K \sim D_S \cdot t^\nu, \quad (\text{F34})$$

with D_S being the initial energy scale where the singlet regime is justified.

ν does not appear to be a universal constant, as it depends on $\alpha = 2\rho_z - 2\rho_z^2$, as shown in Fig. 9(b). A possible explanation is that α may flow to a fixed point at higher orders of ζ_x , in which case ν at that fixed point would be a universal constant. Nevertheless, within a reasonable range of α , $0.2 \leq \alpha \leq 0.5$, ν is approximately 2, consistent with numerical results in the End Matter.

Refs. [111, 115, 116] numerically studied the second order phase transition between a local singlet state and a Kondo Fermi liquid in Anderson models, where the critical exponent ν was found approximately 2. Similar phase transitions [121, 122] have also been suggested in two-impurity models, where the competition between RKKY interaction and Kondo screening drives the critical behavior [117–122].

G. Spectral function and interacting self-energy ansatz in the AD and LS phases

In this section, we discuss the spectral function $A_f(\omega) = -\frac{1}{\pi}\text{Im}G_f(\omega + i0^+)$ in the AD and LS phases. From the analytic form of A_f and G_f , we also construct an ansatz for the interacting self-energy $\Sigma_f(\omega + i0^+)$, which will be an extension of the Hubbard-I approximation (HIA) [131, 132] to capture the low-energy spectral function at and below $\mathcal{O}(J_{S,D})$.

1. Spectral function $A_f(\omega)$

Following Sec. B 5, we first analyze the form of the physical f -electron operator $\tilde{f}_{+\uparrow}^\dagger$ when probed in the *effective* (namely, SW-transformed) models at various energy scales. Then, we analytically calculate $A_f(\omega)$ for $\omega \ll \mathcal{O}(J_{S,D})$ using bosonization, where the physics is governed by the fixed point Hamiltonian. By re-introducing a high-energy multiplet to the fixed-point Hamiltonian, we also demonstrate the formation of the pseudogap shoulders at $\omega \sim \mathcal{O}(J_{S,D})$. Since the irrelevant terms dropped from the fixed point Hamiltonian are not negligible at this energy scale, this latter calculation only serves as a qualitative demonstration.

The FL phase is not discussed here, and there will be a quasiparticle peak at zero energy.

AD phase—In the original Anderson model (see Sec. B 1), which includes the charge fluctuation, the f -electron is by definition created by $f_{ls}^\dagger$. Adding or removing one f -electron costs an energy of $\mathcal{O}(U)$, and leads to the upper and lower Hubbard peaks in the spectral function $A_f(\omega)$ at $\omega \approx \pm \frac{U}{2}$, respectively. After lowering the energy scale to $\omega \sim |J_D| \ll U$, we apply the first SW transformation e^{iS} that integrates out the charge fluctuation, obtaining the (anisotropic) U(4) Kondo model (see Sec. B 2). At this stage, following Sec. B 5, we identify the low-energy component of the f -electron as $\tilde{f}_{+\uparrow}^\dagger = \mathbb{P}_2(e^{iS_1}f_{+\uparrow}^\dagger e^{-iS_1})\mathbb{P}_2 \propto [H^{(K)} - H_0^{(K)}, \psi_{+\uparrow}^\dagger(0)]$, where $H^{(K)}$ is the Kondo Hamiltonian and $H_0^{(K)}$ is the Hamiltonian of bath electrons. According to Table IV, we obtain

$$\begin{aligned} \tilde{f}_{+\uparrow}^\dagger &\propto \lambda_z \cdot \Lambda_z \cdot \psi_{+\uparrow}^\dagger + \zeta_x \sqrt{2} \cdot \Theta_+ \cdot \psi_{-\uparrow}^\dagger \\ &+ \zeta_{0z} \cdot \left(\Theta^{0z} \cdot \psi_{+\uparrow}^\dagger + (\Theta^{0x} + i\Theta^{0y}) \cdot \psi_{+\downarrow}^\dagger \right) + \zeta_{zz} \cdot \left(\Theta^{zz} \cdot \psi_{+\uparrow}^\dagger + (\Theta^{zx} + i\Theta^{zy}) \cdot \psi_{+\downarrow}^\dagger \right) \\ &+ \zeta_{xz} \cdot \left((\Theta^{xz} + i\Theta^{yz}) \psi_{-\uparrow}^\dagger + (\Theta^{xx} + i\Theta^{xy} + i\Theta^{yx} - \Theta^{yy}) \cdot \psi_{-\downarrow}^\dagger \right). \end{aligned} \quad (\text{G1})$$

We have omitted the particle-hole breaking couplings $\gamma_{S,D,T}$ as they are irrelevant in the low-energy physics. The $\Theta^{\mu\nu}$ and Λ_z operators are defined in Sec. B 2 and $\Theta_+ = |S\rangle\langle D, 2| + |D, 2\rangle\langle S|$. According to Table IV, the ζ_x term represents the multiplet fluctuation from D to S , and the ζ_{xz} term represents the multiplet fluctuation from D to T , hence correspond to excitations upon the ground states that involve the D manifold. They will lead to the shoulders of the pseudogap in $A_f(\omega)$ at the energy scale of $\omega \approx \pm |E_S - E_D|, \pm |E_T - E_D|$, respectively. ζ_{0z} and ζ_{zz} , on the other hand, act within the $S \oplus T$ manifold, and will annihilate the ground D states.

To further integrate out the multiplet fluctuation away from the D manifold, we need to apply a second SW transformation $e^{iS'}$, and arrive at the final low-energy theory described by the pair-Kondo model (Eq. (B26)). At this stage, we identify the low-energy f -component as $\tilde{f}_{+\uparrow}^\dagger = \mathbb{P}_D(e^{iS'}\mathbb{P}_2(e^{iS}f_{+\uparrow}^\dagger e^{-iS})\mathbb{P}_2 e^{-iS'})\mathbb{P}_D \propto [H_{\text{PK}} - H_{\text{PK},0}, \psi_{+\uparrow}^\dagger(0)]$, where $H_{\text{PK},0}$ is the bath Hamiltonian in the pair-Kondo model. We find

$$\tilde{f}_{+\uparrow}^\dagger \propto \lambda_z \cdot \Lambda_z \cdot \psi_{+\uparrow}^\dagger + (2\pi\lambda_x x_c) \cdot \Lambda_+ \cdot \psi_{-\uparrow}^\dagger \psi_{-\downarrow}^\dagger \psi_{+\downarrow} \quad (\text{G2})$$

Notice that $H_{\text{PK}} - H_{\text{PK},0}$, as discussed in Sec. B 3, may contain terms of the form of $\mathbb{P}_D \cdot \psi^\dagger \psi^\dagger \psi \psi$, $\Lambda_z \cdot \psi^\dagger \psi^\dagger \psi \psi$, which leads to components like $\mathbb{P}_D \cdot \psi^\dagger \psi^\dagger \psi$ and $\Lambda_z \cdot \psi^\dagger \psi^\dagger \psi$ in $\tilde{f}_{+\uparrow}^\dagger$. Nevertheless, as irrelevant perturbations, they only lead to a smooth ω^2 correction in the low-energy regime besides the major contributions from Eq. (G2), as will be clear soon.

Next, we compute the Green's function of $\tilde{f}_{+\uparrow}^\dagger$ in the AD phase using the fixed point Hamiltonian,

$$H = \int \frac{dx}{4\pi} \sum_{\chi=c,s,v,vs} : (\partial_x \phi_\chi(x))^2 : + 2\rho_z \Lambda_z \cdot \partial_x \phi_v(x) - J_D \cdot \mathbb{P}_D - J_S \cdot \mathbb{P}_S \quad (\text{G3})$$

In order to demonstrate how the multiplet fluctuation to S can lead to the shoulders of the pseudogap, we re-introduced the singlet state $|S\rangle = |0\rangle$ to the model, which has a large energy gap of $J_S - J_D$ above the D manifold. The transverse couplings (PK coupling) within the D manifold λ_x has flowed to 0 at the fixed point, and the transverse coupling between the S and D

manifolds ζ_x is also assumed to be 0 at the fixed point. With PHS, $\mathbb{P}_S$ cannot couple to any fermion bilinear terms, while the quartic couplings are ignored.

To solve Eq. (G3), as we have done around Eq. (B39) in Sec. B3, we apply a gauge transformation $U = e^{i2\rho_z \Lambda_z \phi_v(0)}$, after which the bath and the impurity completely decouple

$$\overline{H} = U H U^\dagger = \int \frac{dx}{4\pi} \sum_{\chi=c,s,v,vs} : (\partial_x \phi_\chi(x))^2 : - J'_D \mathbb{P}_D - J_S \mathbb{P}_S \quad (\text{G4})$$

Here, $J'_D = J_D + \frac{4\rho_z^2}{x_c}$ absorbs the energy correction due to the coupling in the D sector $-\frac{4\rho_z^2}{x_c} \Lambda_z^2 = -\frac{4\rho_z^2}{x_c} \mathbb{P}_D$. We now define $J = J'_D - J_S$ as the multiplet excitation energy to the S manifold.

As the fixed point Hamiltonian, Eq. (G2) faithfully describes the $\tilde{f}$ -operator in the PK energy scale $\omega \ll \mathcal{O}(J)$. We dub the two components as $\tilde{f}_{+\uparrow}^{(1)\dagger} \propto \Lambda_z \cdot \psi_{+\uparrow}^\dagger$, $\tilde{f}_{+\uparrow}^{(2)\dagger} \propto \Lambda_+ \cdot \psi_{-\uparrow}^\dagger \psi_{-\downarrow}^\dagger \psi_{+\downarrow}$. According to Eq. (G1), the $\tilde{f}$ -operator should also incorporate an component $\tilde{f}_{+\uparrow}^{(3)\dagger} \propto \Theta_+ \cdot \psi_{-\uparrow}^\dagger$ at energy scale $\mathcal{O}(J)$, which excites the D states to the S states. At the fixed point Hamiltonian, the impurity $U(1)_v$ charge, which distinguishes between the three impurity states, $|D, 2\rangle$, $|D, \bar{2}\rangle$, and $|S\rangle$, and the bath charges of each flavor ls are separately conserved. Thus, there will be no cross terms between the correlation functions of the three components above as they carry different charges. We now compute them individually.

After $U = e^{i2\rho_z \Lambda_z \phi_v(0)}$, the three components are transformed into

$$U \left(\tilde{f}_{+\uparrow}^{(1)\dagger} \right) U^\dagger \propto \Lambda_z \cdot F_{+\uparrow}^\dagger \cdot e^{i\left(\frac{\phi_c}{2}(0) + \frac{\phi_s}{2}(0) + \frac{\phi_v}{2}(0) + \frac{\phi_{vs}}{2}(0)\right)} \quad (\text{G5})$$

$$U \left(\tilde{f}_{+\uparrow}^{(2)\dagger} \right) U^\dagger \propto \Lambda_+ \cdot F_{-\uparrow}^\dagger F_{-\downarrow}^\dagger F_{+\downarrow} \cdot e^{\frac{1}{2}\phi_c(0)} e^{\frac{1}{2}\phi_s(0)} e^{\frac{1}{2}\phi_{vs}(0)} e^{-i\left(\frac{3}{2} - 4\rho_z\right)\phi_v(0)} \quad (\text{G6})$$

$$U \left(\tilde{f}_{+\uparrow}^{(3)\dagger} \right) U^\dagger \propto \Theta_+ \cdot F_{-\uparrow}^\dagger \cdot e^{\frac{1}{2}\phi_c(0)} e^{\frac{1}{2}\phi_s(0)} e^{-\frac{1}{2}\phi_{vs}(0)} e^{-i\left(\frac{1}{2} - 2\rho_z\right)\phi_v(0)} \quad (\text{G7})$$

where we have exploited $[\Lambda_z, \Theta_+] = \Theta_+$, $[\Lambda_z, \Lambda_+] = 2\Lambda_+$ and hence $U\Theta_+U^\dagger = \Theta_+ e^{i2\rho_z \phi_v(0)}$, $U\Lambda_+U^\dagger = \Lambda_+ e^{i4\rho_z \phi_v(0)}$. Then, according to the correlation functions in Eqs. (A61) and (A62), the imaginary-time Green's function for $\tilde{f}^{(1)\dagger}$ in the $T \rightarrow 0^+$ limit reads

$$G_f^{(1)}(\tau) = -\left\langle T_\tau e^{\tau H} \left(\tilde{f}_{+\uparrow}^{(1)} \right) e^{-\tau H} \cdot \left(\tilde{f}_{+\uparrow}^{(1)\dagger} \right) \right\rangle_0 \sim -\langle \Lambda_z^2 \rangle \left[\theta(\tau) \frac{x_c}{|\tau|} - \theta(-\tau) \frac{x_c}{|\tau|} \right]. \quad (\text{G8})$$

As Λ_z commutes with the Hamiltonian, it produces a factor Λ_z^2 , whose average can be factored out, and produces $\langle \Lambda_z^2 \rangle = 1$ in the D manifold. The remaining correlation function is then identical to the correlation function of a bath electron $\psi_{+\uparrow}^\dagger(0)$, which decays as $\frac{1}{\tau}$, and corresponds to a constant density of states across all ω . Correspondingly, $G_f^{(1)}(\omega)$ contributes a constant background in $A_f(\omega)$,

$$A_f^{(1)}(\omega) \propto \text{const}. \quad (\text{G9})$$

For $\tilde{f}^{(2)\dagger}$, as $\Lambda_\pm$ commutes with $\overline{H}$ (because $\Lambda_\pm$ commutes with both $\mathbb{P}_D = \Lambda_z^2$ and $\mathbb{P}_S$), the Green's function is simply determined by the remaining vertex operators of bath fields. According to Eqs. (A59), (A61) and (A62), we obtain

$$G_f^{(2)}(\tau) = -\left\langle e^{\tau H} \left(\tilde{f}_{+\uparrow}^{(2)} \right) e^{-\tau H} \cdot \tilde{f}_{+\uparrow}^{(2)\dagger} \right\rangle_0 \sim -\left[\theta(\tau) \left(\frac{x_c}{|\tau|} \right)^{\alpha_2} - \theta(-\tau) \left(\frac{x_c}{|\tau|} \right)^{\alpha_2} \right] \quad (\text{G10})$$

where the power $\alpha_2 = \frac{3}{4} + \left(\frac{3}{2} - 4\rho_z\right)^2$. Following the same trick of contour integral of irrational functions used in Sec. C2, the corresponding spectral function should be

$$A_f^{(2)}(\omega) \sim x_c^{\alpha_2} |\omega|^{\alpha_2 - 1} \quad (\text{G11})$$

Importantly, for $0 < \rho_z < \rho_z^c = \frac{1}{2} - \frac{1}{2\sqrt{2}} \approx 0.1464$, $2 > \alpha_2 - 1 > 0.5858$, so $A_f^{(2)}$ can either behave as a smooth dip (if ρ_z is small, so that $\alpha_2 - 1 > 1$), or a kink downward (if ρ_z is large and approaches the BKT critical value, so that $\alpha_2 - 1 < 1$). Added up, $A_f^{(1)} + A_f^{(2)}$ determines the spectral features at low frequency $\omega \ll \mathcal{O}(J)$.

Finally, we compute the Green's function for $\tilde{f}^{(3)}$, which contains a multiplet excitation to the S manifold,

$$G_f^{(3)}(\tau) = -\left\langle T_\tau \cdot e^{\tau H} \left(\tilde{f}_{+\uparrow}^{(3)} \right) e^{-\tau H} \cdot \tilde{f}_{+\uparrow}^{(3)\dagger} \right\rangle_0 \quad (\text{G12})$$

$$\propto -\left\langle T_\tau \cdot e^{\tau \overline{H}} \left(\Theta_- \cdot e^{-i\frac{\phi_c(0)}{2}} e^{-i\frac{\phi_s(0)}{2}} e^{i\frac{\phi_{vs}(0)}{2}} e^{i\left(\frac{1}{2} - 2\rho_z\right)\phi_v(0)} \right) e^{-\tau \overline{H}} \cdot \left(\Theta_+ \cdot e^{i\frac{\phi_c(0)}{2}} e^{i\frac{\phi_s(0)}{2}} e^{-i\frac{\phi_{vs}(0)}{2}} e^{-i\left(\frac{1}{2} - 2\rho_z\right)\phi_v(0)} \right) \right\rangle_0.$$

Crucially, the S sector is higher by an energy of J than the D sector. Therefore, if $\tau > 0$, the time-evolution operator $e^{\tau\bar{H}}$ lives in the D sector, while $e^{-\tau\bar{H}}$ lives in the S sector, as it is sandwiched by Θ_- and Θ_+ , leading to a $e^{-\tau J}$ factor. On the other hand, if $\tau < 0$, $e^{-\tau\bar{H}}$ will live in the D sector, while $e^{\tau\bar{H}}$ will live in the S sector, leading to a $e^{\tau J}$ factor. By also computing the bath correlations, which is directly determined by the total scaling dimension $\alpha_3 = \frac{3}{4} + (\frac{1}{2} - 2\rho_z)^2$, we obtain

$$G_f^{(3)}(\tau) \sim - \left[\theta(\tau) \left(\frac{x_c}{|\tau|} \right)^{\alpha_3} e^{-\tau|J|} - \theta(-\tau) \left(\frac{x_c}{|\tau|} \right)^{\alpha_3} e^{\tau|J|} \right]. \quad (\text{G13})$$

The Mastubara Green's function is given by $G(i\omega) = \int_{-\infty}^{\infty} d\tau G(\tau) e^{i\omega\tau}$. Following the same trick of contour integral of irrational functions used in Sec. C2, where $f(z)$ should be chosen as $(J - i\omega)^{\alpha_3-1}$ and it has a branch-cut at $z = -iy$ ($y \geq J$) (Fig. 6). We obtain

$$G_f^{(3)}(i\omega) = -x_c^{\alpha_3} \cdot \Gamma(1-\alpha_3) \cdot \left((J - i\omega)^{\alpha_3-1} - (J + i\omega)^{\alpha_3-1} \right) \quad (\text{G14})$$

$$G_f^{(3)}(\omega + i0^+) = -x_c^{\alpha_3} \cdot \Gamma(1-\alpha_3) \cdot \left((J - \omega - i0^+)^{\alpha_3-1} - (J + \omega + i0^+)^{\alpha_3-1} \right). \quad (\text{G15})$$

The $(J - \omega - i0^+)^{\alpha_3-1}$ and $(J + \omega + i0^+)^{\alpha_3-1}$ factors in the retarded Green's functions should be interpreted as $f(z = -i\omega + 0^+)$ and $f(z = i\omega - 0^+)$, respectively. According to the branch-cut shown in Fig. 6(b), there are

$$\text{Im}[f(z = -i\omega + 0^+)] = -\sin((\alpha_3 - 1)\pi) \cdot |\omega - J|^{\alpha_3-1} \cdot \theta(\omega - J), \quad (\text{G16})$$

$$\text{Im}[f(z = i\omega - 0^+)] = \sin((\alpha_3 - 1)\pi) \cdot |\omega - J|^{\alpha_3-1} \cdot \theta(-\omega - J). \quad (\text{G17})$$

Thus, the corresponding spectral function is

$$A_f^{(3)}(\omega) \sim x_c^{\alpha_3} \cdot \frac{\pi}{\Gamma(\alpha_3)} \cdot \left(\theta(\omega - J) |\omega - J|^{\alpha_3-1} + \theta(-\omega - J) |\omega + J|^{\alpha_3-1} \right), \quad (\text{G18})$$

where the relation $\Gamma(1 - \alpha_3) \cdot \sin(\pi(1 - \alpha_3)) = \frac{\pi}{\Gamma(\alpha_3)}$ is used. For $0 < \rho_z < \rho_z^c = \frac{1}{2} - \frac{1}{2\sqrt{2}}$, $0 > \alpha_3 - 1 > -0.2071$.

We also remark on the 'irrelevant' components in f , with the form of $\Lambda_z \cdot \psi^\dagger \psi^\dagger \psi$ or $\mathbb{P}_D \cdot \psi^\dagger \psi^\dagger \psi$. As the gauge transformation commutes with Λ_z and $\mathbb{P}_D = \Lambda_z^2$, it does not alter the scaling dimension of these components, hence the time-decaying power α is completely determined by the bath fields, which will be $\alpha = 3$. The corresponding spectral function must be proportional to ω^2 , i.e.,

$$A_f^{(4)}(\omega) \sim x_c^3 \omega^2, \quad (\text{G19})$$

which is negligible compared to $A_f^{(1)} + A_f^{(2)}$ in the low-energy regime.

$A_f^{(1)}(\omega) + A_f^{(2)}(\omega) + A_f^{(3)}(\omega) + A_f^{(4)}(\omega)$ sketches the basic features of the spectral function in the AD phase: $A_f^{(1)}(\omega)$ gives a constant spectral weight around $\omega = 0$, $A_f^{(2)}(\omega)$ gives a kink at $\omega = 0$ when the system is close to the BKT transition point, and $A_f^{(3)}(\omega)$ qualitatively reproduces the pseudogap shoulders at the multiplet excitation energy. As has been remarked, since the fixed point Hamiltonian is only valid at energy scales far below $\mathcal{O}(J_{S,D})$, only $A_f^{(1,2)}(\omega)$ are quantitatively reliable at $\omega \ll J_{S,D}$. $A_f^{(3)}(\omega)$, on the other hand, corresponds to features at $\omega \sim J_{S,D}$, and only qualitatively demonstrates that the shoulder peaks are contributed by excitations like $\Theta_+ \cdot \psi^\dagger$.

LS phase—To understand the LS phase, similarly, we can carry out another second SW transformation $e^{iS''}$ that integrates out the multiplet fluctuation away from the S manifold. In the final low-energy theory, the only impurity operator that can be written is $\mathbb{P}_S$, which cannot couple to any bilinear bath operator, if assuming PHS (see Sec. B2). However, the second SW transformation can lead to quartic couplings of the form $\mathbb{P}_S \cdot \psi^\dagger \psi^\dagger \psi \psi$ (similar to discussions in Sec. B3), namely, an effective interaction of the bath electrons at the spatial origin $x = 0$. The form of this effective interaction will be calculated in Sec. H2, and such a quartic terms will be verified as irrelevant at the LS fixed point. Nevertheless, it brings about the following components of the quasiparticle operator $\tilde{f}_{+\uparrow}^{(4)\dagger} \propto \mathbb{P}_S \cdot \psi_{+\uparrow}^\dagger \psi_{l\uparrow}^\dagger \psi_{l\downarrow}$, $\tilde{f}_{+\uparrow}^{(5)\dagger} \propto \mathbb{P}_S \cdot \psi_{-\uparrow}^\dagger \psi_{+\downarrow}^\dagger \psi_{-\downarrow}$. Such operators all possess scaling dimension $\alpha = 3$, hence contribute a quadratic term in the spectral function (Eq. (G19)).

In order to demonstrate the formation of pseudogap, we also re-introduce the D manifold, and consider the fixed point Hamiltonian (obtained in Sec. F, rewritten in the following form by using $\phi_v = \frac{\varphi_\uparrow + \varphi_\downarrow}{\sqrt{2}}$, and noting that $\phi_{vs} = \frac{\varphi_\uparrow - \varphi_\downarrow}{\sqrt{2}}$ decouples).

$$H = \int \frac{dx}{4\pi} : (\partial_x \phi_v)^2 : + \frac{\varepsilon_D}{x_c} \cdot \mathbb{P}_D + 2\rho_z \Lambda_z \cdot \partial_x \phi_v(x) \Big|_{x=0} \quad (\text{G20})$$

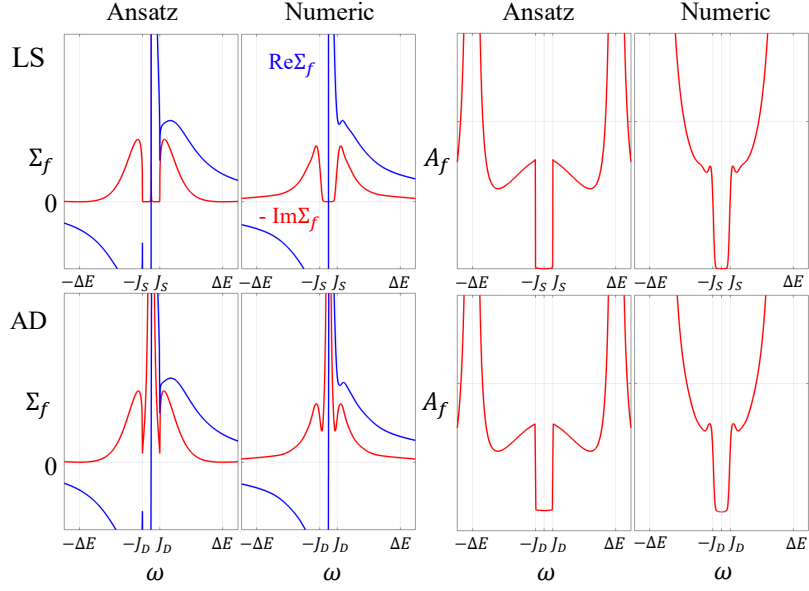


FIG. 10. Ansatz for interacting self-energy $\Sigma_f(\omega + i0^+)$, compared with NRG result. We have absorbed the on-site potential ϵ_f to cancel the Hartree-Fock value of $\Sigma_f(\omega + i0^+)$. We choose $U = 3$ and $\Delta_0 = 0.04$ for the Anderson model parameters. (Upper) For the LS phase, the anti-Hund's couplings are chosen as $J_S = 0.2$, $J_D = 0$. The parameters in the analytical ansatz are $\beta_3 = 0.15$, $D_3 = 7J_S$. (Lower) For the AD phase, $J_S = 0$, $J_D = 0.2$. The tuning parameters adopted in the analytical ansatz are $\beta_1 = \beta_2 = 0.03$, $\beta_3 = 0.12$, $D_1 = D_2 = D_3 = 7J_D$, and $\alpha_2 = 1.9$. In the atomic limit, the peaks in the spectral density experience weak hybridization-induced broadening, so we keep more multiplets (8000) and use a larger $n_z = 8$ than the default choice to better resolve the spectral function.

By similarly applying the gauge transformation $U = e^{i2\rho_z\phi_v(0)}$, the D sector also decouples from the bath,

$$\bar{H} = \int \frac{dx}{4\pi} : (\partial_x \phi_v)^2 : + \frac{\varepsilon'_D}{x_c} \cdot \mathbb{P}_D \quad (\text{G21})$$

where $\varepsilon'_D = \varepsilon_D - 4\rho_z^2 > 0$. Eq. (G21) is identical to Eq. (G4), except with the sign of ε_D reversed, so that the S multiplet becomes the ground state. We can now compute the spectral function due to excitations like $\tilde{f}_{+\uparrow}^{(3)\dagger} \propto \Theta_+ \cdot \psi_{-\uparrow}^\dagger$. $U\tilde{f}^{(3)\dagger}U^\dagger$ follows identically as Eq. (G7) after the gauge transformation, and hence in the LS phase, the Green's function of $\tilde{f}^{(3)\dagger}$ has the same expression as Eq. (G12). The only difference is that $\bar{0}$ is in the S manifold, instead of D , but all the other derivation follows identically. Finally, we arrive at $A_f^{(3)}$ in Eq. (G18), with J given by $\frac{\varepsilon'_D}{x_c}$.

$A^{(3)}(\omega) + A_f^{(4)}(\omega)$ sketches the basic features of the spectral function in the LS phase.

We finally remark that, without PHS, there can be a term of $\mathbb{P}_S \cdot \psi^\dagger \sigma^0 \zeta^0 \psi$ in $[H - H_0]$, hence there will be a component proportional to $\mathbb{P}_S \cdot \psi^\dagger$ in the definition of $\tilde{f}^\dagger$. This term has scaling $\alpha = 1$, and will lead to a finite constant background in $A_f(\omega)$ at $\omega = 0$.

2. Ansatz for interacting self-energy $\Sigma_f(\omega + i0^+)$

In the original Anderson problem with the constant hybridization function Δ_0 (see Sec. B 1), the retarded Green's function of f electron and the interacting self-energy $\Sigma_f(\omega + i0^+)$ are related by

$$G_f(\omega + i0^+) = \frac{1}{\omega - \Sigma_f(\omega + i0^+) + i\Delta_0}, \quad (\text{G22})$$

where the on-site potential ϵ_f is absorbed into Σ_f . Now that we have an analytical understanding to the low-energy features in $A_f(\omega)$ ($\omega \ll \mathcal{O}(U)$), while we already know that the high-energy behavior is dominated by the Hubbard bands ($\omega \sim \mathcal{O}(U)$), we are able to construct an analytical ansatz for the interacting self-energy $\Sigma_f(\omega + i0^+)$, with the aim to reproduce $A_f(\omega)$ in the full energy range. With such an ansatz of Σ_f , one can also easily calculate the lattice spectral function $A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} \frac{1}{\omega - H(\mathbf{k}) - \Sigma_f(\omega + i0^+)}$, where $H(\mathbf{k})$ is the lattice Bloch Hamiltonian, within the framework of dynamical mean-field theory (DMFT). Our ansatz of Σ_f will be an extension to HIA, which only reproduces the Hubbard bands in the high-energy end.

Let us start with the high-energy end $\omega \sim \mathcal{O}(U)$, where the main feature of G_f , the Hubbard peaks, is already captured by HIA. HIA approximates the interacting self-energy as the “atomic” one $\Sigma_f^{(\text{at})}(\omega + i0^+) = \omega - \left(G_f^{(\text{at})}(\omega + i0^+)\right)^{-1}$, where $G_f^{(\text{at})}$ is the Green’s function of f electron computed for an isolated impurity (an “atom”) [131],

$$G_f^{(\text{at})}(\omega + i0^+) = \frac{1}{Z} \sum_{\Xi, \Xi_0} \frac{|\langle \Xi | f_{ls} | \Xi_0 \rangle|^2}{\omega + E_\Xi - E_{\Xi_0} + i0^+} + \frac{1}{Z} \sum_{\Xi} \frac{|\langle \Xi | f_{ls}^\dagger | \Xi_0 \rangle|^2}{\omega + E_{\Xi_0} - E_\Xi + i0^+} \quad (\text{G23})$$

The above expression is at low-temperature limit $T \ll J_{S,D}$. Here, Ξ_0 runs over the impurity ground states, and Z is the impurity ground state degeneracy - in AD, $\Xi_0 \in D$ and $Z = 2$, and in LS, $\Xi_0 \in S$ and $Z = 1$. Ξ represents impurity excited states, with $E_\Xi - E_{\Xi_0} \geq 0$. From Eq. (G23), one can easily read off that, removing one f electron contributes a pole at negative frequency ω , while adding one electron contributes a pole at positive frequency ω . Since all flavors ls are degenerate, the result will be equal for all ls . For the current model at PHS, for both AD and LS, there will be

$$G_f^{(\text{at})}(\omega + i0^+) = \frac{1}{2} \frac{1}{\omega + \Delta E + i0^+} + \frac{1}{2} \frac{1}{\omega - \Delta E + i0^+} = \frac{\omega + i0^+}{(\omega + i0^+)^2 - (\Delta E)^2} \quad (\text{G24})$$

where $\Delta E \approx \frac{U}{2}$. Directly inverting this Green’s function, one obtains the HIA ansatz of interacting self-energy,

$$\Sigma_f^{(\text{at})}(\omega + i0^+) = \frac{(\Delta E)^2}{\omega + i0^+} \quad (\text{G25})$$

For this PHS result, $\Sigma_f^{(\text{at})}$ has a pole at $\omega = 0$. Notice that the spectral function of $A_f^{(\text{at})}(\omega) = -\frac{1}{\pi} \text{Im} G_f^{(\text{at})}(\omega + i\eta)$ is already normalized, namely, $1 = \int d\omega A_f^{(\text{at})}(\omega)$.

Besides the poles at $\pm \Delta E$, the asymptotic behaviors of $G_f^{(\text{at})}$ include

$$G_f^{(\text{at})}(\omega + i0^+) \xrightarrow{\omega \rightarrow 0} -\frac{\omega}{(\Delta E)^2} + \dots, \quad G_f^{(\text{at})}(\omega + i0^+) \xrightarrow{\omega \rightarrow \infty} \frac{1}{\omega} + \dots \quad (\text{G26})$$

LS phase—Next we add the pseudogap at $\mathcal{O}(J)$. As discussed in the previous section, the non-universal power-law singularities at $\omega \sim \mathcal{O}(J)$ need not be treated as quantitatively valid features. Also, in the true ‘atomic’ limit, we expect $\alpha_3 \rightarrow 1$ as $\rho_z \rightarrow 0$, where the singularity becomes rather weak. Therefore, for simplicity and for practical convenience, we simply set $\alpha_3 = 1$. Meanwhile, we impose a smooth cutoff with width $D_3 \sim J$, in order to describe the fact that the $\tilde{f}^{(3)}$ component is not well-defined at arbitrary energy scale, but only within some range near $\mathcal{O}(J)$.

$$A_f^{(3)}(\omega) = \frac{1}{2 \arctan \frac{D_3}{J}} \frac{D_3}{\omega^2 + D_3^2} \left[\theta(-J - \omega) + \theta(\omega - J) \right] \quad (\text{G27})$$

Here, we have attached a constant to guarantee the normalization that $1 = \int d\omega A_f^{(3)}(\omega)$, which can be quickly verified from

$$\int_{-\infty}^{-J} d\omega \frac{D_3}{\omega^2 + D_3^2} + \int_J^{\infty} d\omega \frac{D_3}{\omega^2 + D_3^2} = 2 \arctan \frac{D_3}{J} \quad (\text{G28})$$

Next, we compute the real-part of the Green’s function corresponding to $A_f^{(3)}(\omega)$, from the Kramer-König relation,

$$\begin{aligned} G_f^{(3)}(\omega + i0^+) &= \int_{-\infty}^{\infty} d\epsilon \frac{A_f^{(3)}(\epsilon)}{\omega + i0^+ - \epsilon} = \frac{1}{2 \arctan \frac{D_3}{J}} \left[\int_{-\infty}^{-J} d\epsilon + \int_J^{\infty} d\epsilon \right] \frac{1}{\omega + i0^+ - \epsilon} \frac{D_3}{\epsilon^2 + D_3^2} \\ &= \frac{1}{2 \arctan \frac{D_3}{J}} \left(-\frac{D_3}{\omega^2 + D_3^2} \ln \frac{\epsilon - (\omega + i0^+)}{D} + \frac{i}{2} \frac{1}{\omega + iD_3} \ln \left(\frac{\epsilon + iD_3}{D_3} \right) - \frac{i}{2} \frac{1}{\omega - iD_3} \ln \left(\frac{\epsilon - iD_3}{D_3} \right) \right) \left(\left[-\infty \right] + \left[J \right] \right) \\ &= \frac{1}{2 \arctan \frac{D_3}{J}} \frac{D_3}{\omega^2 + D_3^2} \ln \frac{J - (\omega + i0^+)}{J + (\omega + i0^+)} + \frac{\omega}{\omega^2 + D_3^2} \end{aligned} \quad (\text{G29})$$

Notice that, with the second term, the poles at $\omega = \pm iD_3$ introduced by the artificial Lorentzian envelope have been canceled.

We choose the interacting self-energy ansatz as

$$\Sigma_f(\omega + i0^+) = \omega - \left(\beta_{\text{at}} G_f^{(\text{at})}(\omega + i0^+) + \beta_3 G_f^{(3)}(\omega + i0^+) \right)^{-1} \quad (\text{G30})$$

where $\beta_{\text{at}} + \beta_3 = 1$ are tuning parameters. Notice that, a $A \sim \omega^2$ component in the spectral function will be automatically generated using the above ansatz of self-energy, which further justifies omitting $A_f^{(4)}$ (Eq. (G19)) in the construction.

The Lorentz truncation function $\frac{D_3^2}{\omega^2 + D_3^2}$ leads to an artifact of the self-energy at $\omega \rightarrow \infty$. According to the Lehmann spectral representation, the correlated self-energy must vanish in the $\omega \rightarrow \infty$ limit. However, since $G_f = \frac{1}{\omega} - i\frac{D_3}{\omega^2} + \dots$, the self-energy has a finite imaginary part in the $\omega \rightarrow \infty$ limit:

$$\Sigma(\omega + i0^+) = \omega - (G_f)^{-1} \sim \omega - \frac{1}{\frac{1}{\omega} - i\frac{D_3}{\omega^2}} \sim \omega - \frac{\omega}{1 - i\frac{D_3}{\omega}} \sim -iD_3. \quad (\text{G31})$$

One may use a faster-decaying truncation function, *e.g.*, $\frac{D_3^3}{\omega^4 + D_3^4}$, to avoid this artifact.

AD phase—We also consider

$$A_f^{(1)}(\omega) = \frac{1}{\pi} \frac{D_1}{\omega^2 + D_1^2} \quad (\text{G32})$$

$$A_f^{(2)}(\omega) = \frac{\sin \frac{\pi\alpha_2}{2}}{\pi D_2^{\alpha_2-2}} \frac{1}{\omega^2 + D_2^2} |\omega|^{\alpha_2-1} \quad (\text{G33})$$

D_1 and D_2 are parameters representing the energy scale where $\tilde{f}^{(1)}$ and $\tilde{f}^{(2)}$ are justified. The normalization of $A_f^{(1)}$ is obvious. For $\alpha_2 < 2$, with which $A_f^{(2)}(\omega)$ exhibits a kink at $\omega = 0$, $A_f^{(2)}$ is also normalized because $\int_{-\infty}^{\infty} d\omega \frac{|\omega|^{\alpha_2-1}}{\omega^2 + D_2^2} = 2D_2^{\alpha_2-2} \int_0^{\infty} dx \frac{x^{\alpha_2-1}}{x^2 + 1} = \frac{\pi D_2^{\alpha_2-2}}{\sin \frac{\pi\alpha_2}{2}}$ (see calculations around Eq. (G36)). For $\alpha_2 > 2$, $A_f^{(2)}(\omega)$ is not normalized. Nevertheless, $A_f^{(2)}$ in this case is featureless because it is smooth and small around $\omega = 0$, and one may omit it. If one were to keep $A_f^{(2)}(\omega)$ with $\alpha_2 > 2$ in the low-energy physics, one may choose a faster-decaying truncation function, *e.g.*, $\frac{D_2^3}{\omega^4 + D_2^4}$, instead of the Lorentz function.

$G_f^{(1)}$ can be obtained from $G_f^{(3)}$ (Eq. (G29)) by setting $J \rightarrow 0^+$,

$$G_f^{(1)}(\omega + i0^+) = \frac{1}{\omega + iD_1} \quad (\text{G34})$$

where the pole at $\omega = iD_1$ is canceled. $G_f^{(2)}$ is given by

$$\begin{aligned} G_f^{(2)}(\omega + i0^+) &= \int_{-\infty}^{\infty} d\epsilon \frac{A_f^{(2)}(\epsilon)}{\omega + i0^+ - \epsilon} = \frac{\sin \frac{\pi\alpha_2}{2}}{\pi D_2^{\alpha_2-2}} \int_{-\infty}^{\infty} d\epsilon \frac{1}{\omega + i0^+ - \epsilon} \frac{|\epsilon|^{\alpha_2-1}}{\epsilon^2 + D_2^2} = \frac{\sin \frac{\pi\alpha_2}{2}}{\pi D_2^{\alpha_2-2}} \int_0^{\infty} d\epsilon \frac{2\omega}{(\omega + i0^+)^2 - \epsilon^2} \frac{\epsilon^{\alpha_2-1}}{\epsilon^2 + D_2^2} \\ &= \frac{\sin \frac{\pi\alpha_2}{2}}{\pi D_2^{\alpha_2-2}} \cdot \frac{2\omega}{\omega^2 + D_2^2} \int_0^{\infty} d\epsilon \left(\frac{\epsilon^{\alpha_2-1}}{\epsilon^2 + D_2^2} + \frac{\epsilon^{\alpha_2-1}}{(\omega + i0^+)^2 - \epsilon^2} \right) \end{aligned} \quad (\text{G35})$$

For $0 < \nu < \mu$, there are

$$\int_0^{\infty} dx \frac{x^{\mu-1}}{x^{\nu} + 1} = \frac{\pi}{\nu} \frac{1}{\sin \frac{\pi\mu}{\nu}} \quad \mathcal{P} \int_0^{\infty} dx \frac{x^{\mu-1}}{1 - x^{\nu}} = \frac{\pi}{\nu} \cot \frac{\pi\mu}{\nu} \quad (\text{G36})$$

Carrying out the principal value integral, we obtain

$$\text{Re}G_f^{(2)}(\omega + i0^+) = \frac{\omega}{\omega^2 + D_2^2} + \frac{\text{sgn}(\omega)}{\omega^2 + D_2^2} \frac{|\omega|^{\alpha_2-1}}{D_2^{\alpha_2-2}} \cos \frac{\pi\alpha_2}{2} \quad (\text{G37})$$

By also matching the imaginary part $\text{Im}G_f^{(2)}(\omega + i0^+) = -\pi A_f^{(2)}(\omega)$, we obtain

$$G_f^{(2)}(\omega + i0^+) = \frac{\omega}{\omega^2 + D_2^2} + \frac{1}{\omega^2 + D_2^2} \cdot \frac{|\omega|^{\alpha_2-1}}{D_2^{\alpha_2-2}} \cdot \left(\cos \frac{\pi\alpha_2}{2} \cdot \text{sgn}(\omega) - i \cdot \sin \frac{\pi\alpha_2}{2} \right). \quad (\text{G38})$$

We can rewrite the factor $|\omega|^{\alpha_2-1} \left(\cos \frac{\pi\alpha_2}{2} \cdot \text{sgn}(\omega) - i \cdot \sin \frac{\pi\alpha_2}{2} \right)$ as

$$\begin{aligned} -i(-i\omega + 0^+)^{\alpha_2-1} &= -i|\omega|^{\alpha_2-1} e^{-i\frac{\pi}{2}(\alpha_2-1)\text{sgn}(\omega)} = -i|\omega|^{\alpha_2-1} \left(\cos \frac{\pi(\alpha_2-1)}{2} - i \cdot \text{sgn}(\omega) \sin \frac{\pi(\alpha_2-1)}{2} \right) \\ &= -i|\omega|^{\alpha_2-1} \left(\sin \frac{\pi\alpha_2}{2} + i \cdot \text{sgn}(\omega) \cos \frac{\pi\alpha_2}{2} \right). \end{aligned} \quad (\text{G39})$$

It is direct to verify that the pole of the first term in $G_f^{(2)}$ at $\omega = iD_2$ is canceled by the second term.

We choose the interacting self-energy ansatz as

$$\Sigma_f(\omega + i0^+) = \omega - \left(\beta_{\text{at}} G_f^{(\text{at})}(\omega + i0^+) + \beta_1 G_f^{(1)}(\omega + i0^+) + \beta_2 G_f^{(2)}(\omega + i0^+) + \beta_3 G_f^{(3)}(\omega + i0^+) \right)^{-1} \quad (\text{G40})$$

where $\beta_{\text{at},1,2,3}$ are tuning parameters and satisfy $\beta_{\text{at}} + \beta_1 + \beta_2 + \beta_3 = 1$.

Let us check the asymptotic behavior of Σ_f in AD at $\omega \rightarrow 0$. The ansatz

$$\begin{aligned} G_f(\omega + i0^+) &= \beta_{\text{at}} G_f^{(\text{at})}(\omega + i0^+) + \beta_1 G_f^{(1)}(\omega + i0^+) + \beta_2 G_f^{(2)}(\omega + i0^+) + \beta_3 G_f^{(3)}(\omega + i0^+) \\ \text{Re} G_f(\omega + i0^+) &= \left(\frac{-\beta_{\text{at}}}{(\Delta E)^2} + \frac{\beta_1}{D_1^2} + \frac{\beta_2}{D_2^2} + \frac{\beta_3}{D_3^2} \right) \omega + \mathcal{O}(\omega^3) + \beta_2 \frac{|\omega|^{\alpha_2-1}}{D_2^{\alpha_2}} \cos \frac{\pi\alpha_2}{2} \text{sgn}(\omega) + \mathcal{O}(\omega^{\alpha_2+1}) \\ \text{Im} G_f(\omega + i0^+) &= - \left(\frac{\beta_1}{D_1} + \mathcal{O}(\omega^2) + \frac{\beta_2 |\omega|^{\alpha_2-1}}{D_2^{\alpha_2}} \sin \frac{\pi\alpha_2}{2} + \mathcal{O}(\omega^{\alpha_2+1}) \right) \end{aligned} \quad (\text{G41})$$

Let us focus on the most singular case, namely, $0.5858 < \alpha_2 - 1 < 1$. Then $\frac{\text{Re} G_f}{\text{Im} G_f} = \mathcal{O}(\omega^{\alpha_2-1})$. Then,

$$\begin{aligned} \text{Im} \Sigma_f(\omega + i0^+) &= -\text{Im}[G_f(\omega + i0^+)]^{-1} = \frac{\text{Im} G_f}{(\text{Re} G_f)^2 + (\text{Im} G_f)^2} = \frac{1}{\text{Im} G_f} + \mathcal{O}(\omega^{2(\alpha_2-1)}) \\ &= -\frac{1}{\frac{\beta_1}{D_1} + \frac{\beta_2 |\omega|^{\alpha_2-1}}{D_2^{\alpha_2}} \sin \frac{\pi\alpha_2}{2} + \mathcal{O}(\omega^2)} = -\frac{D_1}{\beta_1} \left(1 - \frac{\beta_2 D_1 |\omega|^{\alpha_2-1}}{\beta_1 D_2^{\alpha_2}} \right) + \mathcal{O}(\omega^{2(\alpha_2-1)}) \end{aligned} \quad (\text{G42})$$

In Fig. 10, we compare the ansatz self-energy with the numeric ones. Using the ansatz $\Sigma_f(\omega + i0^+)$, we also re-compute the spectral function in presence of the constant hybridization $i\Delta_0$, $A_f(\omega) = -\frac{1}{\pi} \text{Im} G_f(\omega + i\eta) = -\frac{1}{\pi} \text{Im} \frac{1}{\omega - \Sigma_f(\omega + i\eta) + i\Delta_0}$, and compare with the NRG result.

3. Application to MATBG with heterostrain

To be concrete, we exploit the topological heavy fermion basis [47, 51, 61]. The heterostrain tensor (namely, the difference of the strain tensors in the two graphene layers) is given by

$$\mathcal{E} = \begin{pmatrix} \epsilon_+ + \epsilon_- & \epsilon_{xy} \\ \epsilon_{xy} & \epsilon_+ - \epsilon_- \end{pmatrix}. \quad (\text{G43})$$

$(\epsilon_{xy}, \epsilon_-) = -\frac{\nu_G+1}{2}\epsilon(\cos(2\varphi), \sin(2\varphi))$ describes the orientation of the strain field, which stretches in one direction and squeezes in another. $\epsilon_+ = \frac{\nu_G-1}{2}\epsilon$ describes an isotropic expansion. $\nu_G = 0.16$ is the Poisson ratio, linking the two effects. We take $(\epsilon_{xy}, \epsilon_-) = (0, 1)$, and $\epsilon = 0.2\%$ for concreteness, which are typical values in experiments.

The heterostrain shears the moiré Brillouin zone, which is characterized by three vectors,

$$\mathbf{q}_j = \theta \frac{4\pi}{3a_G} \left(\sin \frac{2\pi(j-1)}{3}, -\cos \frac{2\pi(j-1)}{3} \right) + \frac{4\pi}{3a_G} \left(\cos \frac{2\pi(j-1)}{3}, \sin \frac{2\pi(j-1)}{3} \right) \cdot \mathcal{E} \quad j = 1, 2, 3 \quad (\text{G44})$$

where $\theta = 1.05^\circ$ denoting the twist angle, and $a_G = 0.246\text{nm}$ denoting the graphene lattice constant.

Due to the valley and spin degeneracies, we only write down the lattice Green's function in one flavor, the $\eta = +$ valley and $s = \uparrow$ spin. The kinetic Hamiltonian on the lattice consists of

$$H(\mathbf{k}) = H_0(\mathbf{k}) + \delta H_\epsilon(\mathbf{k}) + \delta H_{\text{mf}}(\mathbf{k}) \quad (\text{G45})$$

$H_0(\mathbf{k})$ follows Ref. [47],

$$H_0(\mathbf{k}) = \left(\begin{array}{c|cc|c} 0 & h.c. & 0 & \cdots \\ \hline (\gamma\sigma^0 + v'_*(k_x\sigma^x + k_y\sigma^y))e^{-\frac{\lambda^2|\mathbf{k}|^2}{2}} & 0 & h.c. & \cdots \\ \hline 0 & v_*(k_x\sigma^0 - ik_y\sigma^z) & M\sigma_x & \\ \hline \cdots & \cdots & & \end{array} \right) \quad (\text{G46})$$

where the columns are $(f_{\mathbf{k}1}, f_{\mathbf{k}2}, c_{\mathbf{k}1}, c_{\mathbf{k}2}, c_{\mathbf{k}3}, c_{\mathbf{k}4}, c_{(\mathbf{k}+\mathbf{G})1}, c_{(\mathbf{k}+\mathbf{G})2}, c_{(\mathbf{k}+\mathbf{G})3}, c_{(\mathbf{k}+\mathbf{G})4}, \cdots)^T$. Omitted blocks follow by replacing $c_{(\mathbf{k}+\mathbf{G})b}$ to $c_{(\mathbf{k}+\mathbf{G}')b}$ with $b = 1, 2, 3, 4$. $\mathbf{G}, \mathbf{G}'$ run over moiré reciprocal lattice vectors, spanned by $\mathbf{G}_1 = \mathbf{q}_2 - \mathbf{q}_1$ and $\mathbf{G}_2 = \mathbf{q}_3 - \mathbf{q}_1$. $\gamma = -24.75\text{meV}$, $M = 3.697\text{meV}$, $v_* = -430.3\text{meV}\cdot\text{nm}$, and $v'_* = 162.2\text{meV}\cdot\text{nm}$ [47].

$\delta H_\epsilon(\mathbf{k})$ is the couplings induced by heterostrain,

$$\delta H_\epsilon(\mathbf{k}) = \left(\begin{array}{c|cc|c} M_f(\epsilon_{xy}\sigma^x + \epsilon_- \sigma^y) & h.c. & h.c. & \dots \\ \hline i\gamma' \epsilon_+ \sigma^z & c(\epsilon_{xy}\sigma^x + \epsilon_- \sigma^y) & h.c. & \dots \\ c''(\epsilon_{xy}\sigma^0 - i\epsilon_- \sigma^z) & c'(\epsilon_{xy}\sigma^x + \epsilon_- \sigma^y) & M' \epsilon_+ \sigma^y & \dots \\ \hline \dots & \dots & \dots & \dots \end{array} \right) \quad (\text{G47})$$

where $c = -8750\text{meV}$, $c' = 2050\text{meV}$, $c'' = -3362\text{meV}$, $M_f = 4380\text{meV}$, $\gamma' = -3352\text{meV}$, and $M' = -4580\text{meV}$ [51].

In Refs. [61, 62], it is found that a typical heterostrain at charge-neutrality point (CNP) of MATBG ($\nu = 0$) fully polarizes the f flavors along the “Zeeman” splitting of $M_f(\epsilon_{xy}\sigma^x + \epsilon_- \sigma^y)$. Doped to $\nu > 0$, only the flavors that were empty at CNP remain active, while the occupied flavors remain frozen. We make the same assumption here. From this frozen background, there can be a Fock exchange term at the mean-field level of the form $\Delta(\epsilon_{xy}\sigma^x + \epsilon_- \sigma^y)$, where Δ is of $\mathcal{O}(U)$. Besides, the main effect of the other Coulomb interactions between f and c (terms U_2, W, J, V in Ref. [47]) is to adjust the chemical potential for f and c electrons separately, which we define as $\epsilon_f, \epsilon_{c,1}, \epsilon_{c,3}$, following Ref. [53]. In accordance with the rest of this paper, the chemical potential ϵ_f should be adjusted so that the active flavors lie at the Fermi surface. In sum,

$$\delta H_{\text{mf}}(\mathbf{k}) = \left(\begin{array}{c|cc|c} \epsilon_f \sigma^0 + \Delta(\epsilon_{xy}\sigma^x + \epsilon_- \sigma^y) & & & \dots \\ \hline & \epsilon_{c,1} & & \dots \\ & & \epsilon_{c,2} & \dots \\ \hline \dots & \dots & \dots & \dots \end{array} \right) \quad (\text{G48})$$

We choose $(\Delta + M_f) \frac{\nu_G + 1}{2} \epsilon + \epsilon_f = 0$, in order to align the active f flavors with the Fermi energy. For calculations in the main text and End Matter, we choose $\epsilon_{c,1} = -8\text{meV}$ and $\epsilon_{c,2} = -12\text{meV}$. In Fig. 2(c,d) and Fig. 3(a), we choose $U = 50\text{meV}$, so that Hubbard peaks of active f levels lie at $\pm 25\text{meV}$, and we choose the frozen f levels to lie at $\epsilon_f - (\Delta + M_f) \frac{\nu_G + 1}{2} \epsilon = -50\text{meV}$. In Fig. 3(b), we choose $U = 16\text{meV}$, so that Hubbard peaks of active f levels at $\pm 8\text{meV}$, and we choose the frozen f levels to lie at $\epsilon_f - (\Delta + M_f) \frac{\nu_G + 1}{2} \epsilon = -16\text{meV}$.

Finally, the lattice Green’s function is given by

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} \left(\text{Tr} \left[\frac{1}{(\omega + i0^+) - H(\mathbf{k}) - \Sigma(\omega + i0^+)} \right] \right). \quad (\text{G49})$$

H. Effective interactions

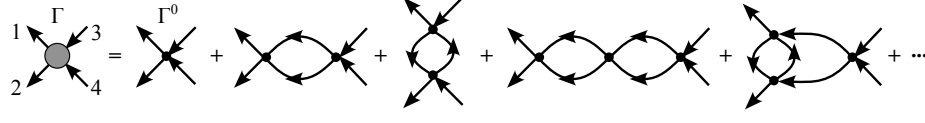
1. Exact asymptotic vertex functions in the FL phase

In this section, we briefly summarize the exact asymptotic relations of the renormalized interactions in the FL phase when $T_K \rightarrow 0^+$. For details about the renormalized perturbation theory, calculation of susceptibilities and Ward identities, we refer the reader to supplementary section B of Ref. [1] and other previous works [92, 94, 97, 111].

In the FL phase, the local Green's function of the f -electron has a quasiparticle peak $\frac{z}{i\omega - \tilde{\epsilon}_f + i\tilde{\Delta}_0(i\omega)}$ contributed by quasiparticle $\tilde{f} \approx z^{-\frac{1}{2}}f$ and an incoherent part, where $z = [1 - \partial_\omega \Sigma_f(\omega)|_{\omega=0}]^{-1}$ is the quasiparticle weight, and $\tilde{\Delta}_0 = z\Delta_0$ is the renormalized hybridization function. The renormalized interactions on the quasiparticles are defined as the zero-frequency value of the full vertex function, scaled by quasiparticle weight:

$$\tilde{U}, \tilde{J}_D, \tilde{J}_S = z^2 \Gamma_{U,D,S}(0, 0; 0, 0) \quad (\text{H1})$$

We have defined the fully anti-symmetrized vertex Γ by



$$\Gamma = \Gamma^0 + \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \dots \quad (\text{H2})$$

where the black dots are the bare interaction Γ^0 and the solid lines are the full Green function. Γ is then separated into different channels by

$$\begin{aligned} \Gamma_{1234} = & \Gamma_U \cdot (\delta_{l_1 l_4} \delta_{l_2 l_3} \delta_{s_1 s_4} \delta_{s_2 s_3} - \delta_{l_2 l_4} \delta_{l_1 l_3} \delta_{s_2 s_4} \delta_{s_1 s_3}) + \Gamma_D \cdot \delta_{l_1 l_2} \delta_{l_2 l_3} \delta_{l_3 l_4} (\delta_{s_1 s_3} \delta_{s_2 s_4} - \delta_{s_1 s_4} \delta_{s_2 s_3}) \\ & + \frac{\Gamma_S}{2} \cdot \delta_{l_1 \bar{l}_2} \delta_{l_3 \bar{l}_4} (\delta_{s_1 s_3} \delta_{s_2 s_4} - \delta_{s_1 s_4} \delta_{s_2 s_3}), \end{aligned} \quad (\text{H3})$$

similar to the bare one (Eq. (B12)).

In general, it is difficult to evaluate the vertex function non-perturbatively. However, in the $T_K \rightarrow 0^+$ limit, when some degrees of freedom of impurity are frozen and symmetry is high enough, we can obtain exact relations about these renormalized parameters. Consider a symmetry generator $\hat{O} = \sum_{ls} f_{ls}^\dagger O_{ls} f_{ls}$ of the system, where the matrix O is assumed diagonal for simplicity. The exact static susceptibility of $\hat{O}$ is related to the vertex function by the Ward identity (supplementary Eq. (B88) of Ref. [1])

$$\chi^O = \frac{\sin \delta_f}{\pi \tilde{\Delta}_0} \cdot \left(\sum_{ls} O_{ls}^2 - \frac{\sin \delta_f}{\pi \tilde{\Delta}_0} \sum_{l_1 s_1 l_2 s_2} z^2 \Gamma_{l_1 s_1, l_2 s_2; l_2 s_2, l_1 s_1}(0, 0; 0, 0) \cdot O_{l_1 s_1} \cdot O_{l_2 s_2} \right). \quad (\text{H4})$$

Here $\delta_f = \frac{n_f}{4}\pi$ and n_f is the filling of the impurity. As we are only interested in the half-filling case ($n_f = 2$), hereafter we set $\sin \delta_f = 1$. We calculate the susceptibilities of charge, spin, and valley $\chi_{c,s,v}$. The corresponding O matrices are $\sigma^0 \zeta^0$, $\sigma^0 \zeta^s$, $\sigma^z \zeta^0$, respectively, and they are indeed generators of the symmetry group $[U(2)_{c,s} \times D_\infty]/\mathbb{Z}_2$. We obtain

$$\chi_c = 4 \frac{1}{\pi \tilde{\Delta}_0} \left[1 - \frac{1}{\pi \tilde{\Delta}_0} \left(3\tilde{U} - \tilde{J}_D - \frac{1}{2}\tilde{J}_S \right) \right] \quad (\text{H5})$$

$$\chi_s = 4 \frac{1}{\pi \tilde{\Delta}_0} \left[1 - \frac{1}{\pi \tilde{\Delta}_0} \left(-\tilde{U} + \tilde{J}_D + \frac{1}{2}\tilde{J}_S \right) \right] \quad (\text{H6})$$

$$\chi_v = 4 \frac{1}{\pi \tilde{\Delta}_0} \left[1 - \frac{1}{\pi \tilde{\Delta}_0} \left(-\tilde{U} - \tilde{J}_D + \frac{1}{2}\tilde{J}_S \right) \right]. \quad (\text{H7})$$

We define the Kondo temperature T_K by $T_K = \tilde{\Delta}_0$ and the above equations yield Eq. (2) in the main text. This definition just differs by an order 1 constant from some other definition of Kondo temperature; for example, Refs. [111, 143] defined $T_K = \frac{\pi}{4}\tilde{\Delta}_0$.

We then consider several limits. For all cases, we let $U \gg T_K$ and n_f is fixed to an integer. We also calculate the effective interactions in S, T, D channel $\tilde{E}_S = \tilde{U} - \tilde{J}_S$, $\tilde{E}_T = \tilde{U}$, $\tilde{E}_D = \tilde{U} - \tilde{J}_D$ (i.e., the two particle energies as calculated in Sec. B 1). They are related to the pairing susceptibility (supplementary section B.5 of Ref. [1]), and a negative two-particle energy indicates an attractive interaction in that channel.

$J_D = J_S = 0, U \gg T_K$ *limit*—This limit enjoys an $SU(4)$ symmetry (Sec. B 1), which enforces $\tilde{J}_D = \tilde{J}_S = 0$. The charge degree of freedom is frozen at the Kondo energy scale, hence χ_c is not contributed by the quasiparticles, implying $\chi_c \ll \tilde{\Delta}_0^{-1}$ and $3\tilde{U} = \pi\tilde{\Delta}_0$. Therefore,

$$(\tilde{U}, \tilde{J}_D, \tilde{J}_S) = \pi\tilde{\Delta}_0 \left(\frac{1}{3}, 0, 0 \right), \quad (\tilde{E}_S, \tilde{E}_T, \tilde{E}_D) = \pi\tilde{\Delta}_0 \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3} \right). \quad (\text{H8})$$

$J_S, J_S - J_D, U \gg T_K$ *limit*—The atomic ground state is the singlet state. As the splittings between the singlet state and other atomic levels are much larger than T_K , in addition to the charge degree of freedom, the spin and valley degrees of freedom are also frozen at the Kondo energy scale, implying $\chi_{c,s,v} \ll \tilde{\Delta}_0^{-1}$. We obtain

$$(\tilde{U}, \tilde{J}_D, \tilde{J}_S) = \pi\tilde{\Delta}_0(1, 0, 4), \quad (\tilde{E}_S, \tilde{E}_T, \tilde{E}_D) = \pi\tilde{\Delta}_0(-3, 1, 1). \quad (\text{H9})$$

Notably, the singlet channel in the renormalized interaction becomes attractive (negative), favoring the singlet pairing.

$J_D, U \gg T_K, J_S = 0$ *limit*—This limit enjoys the $U(2)_+ \times U(2)_-$ symmetry (Sec. B 1), which enforces $\tilde{J}_S = 0$. The atomic ground states are the doublet states, which are spin-singlet, so both $\chi_{c,s}$ are frozen, implying

$$(\tilde{U}, \tilde{J}_D, \tilde{J}_S) = \pi\tilde{\Delta}_0(1, 2, 0), \quad (\tilde{E}_S, \tilde{E}_T, \tilde{E}_D) = \pi\tilde{\Delta}_0(1, 1, -1). \quad (\text{H10})$$

Notably, the doublet channel in the renormalized interaction becomes attractive (negative), favoring the doublet pairing.

$J_S, U \gg T_K, J_S = J_D > 0$ *limit*—This limit enjoys an additional valley $SU(2)_v$ symmetry (Sec. B 1), which enforces $\tilde{J}_S = \tilde{J}_D$. The atomic ground states are the singlet and doublet states, which are valley-triplet and spin-singlet, so we have both $\chi_{c,s}$ frozen, implying

$$(\tilde{U}, \tilde{J}_D, \tilde{J}_S) = \pi\tilde{\Delta}_0 \left(1, \frac{4}{3}, \frac{4}{3} \right), \quad (\tilde{E}_S, \tilde{E}_T, \tilde{E}_D) = \pi\tilde{\Delta}_0 \left(-\frac{1}{3}, 1, -\frac{1}{3} \right). \quad (\text{H11})$$

Notably, the doublet and singlet channels in the renormalized interaction become attractive (negative), favoring the valley-triplet pairing.

$|J_S|, U \gg T_K, J_S = J_D < 0$ *limit*—The $SU(2)_v$ symmetry enforces $\tilde{J}_S = \tilde{J}_D$. The atomic ground states are the triplet states, which are valley-singlet, so we have both $\chi_{c,v}$ frozen, implying

$$(\tilde{U}, \tilde{J}_D, \tilde{J}_S) = \pi\tilde{\Delta}_0 \left(-\frac{1}{3}, -\frac{4}{3}, -\frac{4}{3} \right), \quad (\tilde{E}_S, \tilde{E}_T, \tilde{E}_D) = \pi\tilde{\Delta}_0 \left(1, -\frac{1}{3}, 1 \right). \quad (\text{H12})$$

Notably, the spin-triplet channel in the renormalized interaction becomes attractive (negative), favoring the spin-triplet pairing.

We have sketched those regions with attractive interaction in Fig. 1(b) in the main text. The relations above are verified by the NRG calculation as shown in Fig. 4(b-g) in the End Matter. Eqs. (H8) and (H12) were also obtained in Ref. [94], and Eqs. (H9) and (H10) were also obtained in Ref. [111]. Moreover, Eq. (H11) is equivalent to Eq. (H12) upon interchanging valley and spin.

2. Effective interactions in the LS and AD phases

In the LS and AD phases, the f -quasiparticle has zero quasiparticle weight. Nevertheless, we can still extract the effective interaction by examining energies of two-particle excitations perturbatively.

LS phase—In the LS phase, ζ_x runs towards 0 and ε_D runs towards infinity under the RG. When parameters are close to the fixed point, we can integrate out the high-energy $|\pm 2\rangle$ states to obtain an effective interaction induced by ζ_x . The effective Hamiltonian is given by Eqs. (B45) and (B46) with the renormalized ζ_x, ε_D , and we find it convenient to reverse the process in Sec. B 4 and rewrite it in the fermion Hamiltonian (Eq. (B42)):

$$H^{(S,D)} = \sum_{ls} k : d_{ls}^\dagger(k) d_{ls}(k) : + J \cdot \Lambda_z^2 + (2\pi\lambda_z)\Lambda_z \sum_{ls} l \cdot \psi_{ls}^\dagger(0) \psi_{ls}(0) + (2\pi\zeta_x) \left(\Theta_+ \cdot \sum_s \psi_{-s}^\dagger(0) \psi_{+s}(0) + h.c. \right). \quad (\text{H13})$$

ρ_z as well as λ_z are unchanged under RG. $J = \varepsilon_D + \frac{4\rho_z^2}{x_c}$ is large and we treat ζ_x as perturbatively. Applying the second-order perturbation theory, the correction from the ζ_x term is

$$\begin{aligned} H_{\text{int}}^{(S)} &= (4\pi\zeta_x)^2 \sum_{L_z=2, \bar{2}} \frac{|\langle L^z | (\Theta_+ \cdot \sum_s \psi_{-s}^\dagger(0) \psi_{+s}(0) + h.c.) | 0 \rangle|^2}{-J} \\ &= -\frac{32\pi^2 \zeta_x^2}{J} \sum_{i=x,y} \psi^\dagger(0) \sigma^i \zeta^0 \psi(0) \cdot \psi^\dagger(0) \sigma^i \zeta^0 \psi(0) \end{aligned}$$

We define $\hat{T}^i = \frac{1}{2} \psi^\dagger \sigma^i \zeta^0 \psi$, $\hat{S}^i = \frac{1}{2} \psi^\dagger \sigma^0 \zeta^i \psi$, $\hat{S}_l^i = \frac{1}{2} \psi^\dagger \frac{\sigma^0 + l \cdot \sigma^z}{2} \zeta^i \psi$, $\hat{N} = \psi^\dagger \sigma^0 \zeta^0 \psi$, $\hat{\mathbf{T}} = (\hat{T}^x, \hat{T}^y, \hat{T}^z)$, $\hat{\mathbf{S}} = (\hat{S}^x, \hat{S}^y, \hat{S}^z)$, $\hat{\mathbf{S}}_l = (\hat{S}_l^x, \hat{S}_l^y, \hat{S}_l^z)$ in this section. Making use of the operator identities:

$$\hat{\mathbf{T}}^2 + \hat{\mathbf{S}}^2 + \frac{1}{2}(\hat{N} - 2)^2 = 2, \quad \hat{S}_l^2 = \frac{3}{4} \hat{N}_l (2 - \hat{N}_l), \quad (\text{H14})$$

we have

$$\hat{T}^x \hat{T}^x + \hat{T}^y \hat{T}^y = \hat{\mathbf{T}}^2 - \hat{T}^z \hat{T}^z = -\frac{1}{4} \hat{N}(\hat{N} - 1) + \frac{1}{2} \hat{N} + \frac{1}{2} \sum_l \hat{N}_{l\uparrow} \hat{N}_{l\downarrow} - 2\hat{\mathbf{S}}_+ \cdot \hat{\mathbf{S}}_- . \quad (\text{H15})$$

The effective interaction can be rewritten in a similar form to Eq. (B7):

$$H_{\text{int}}^{(S)} = \epsilon'_f \hat{N} + \left(U' - \frac{1}{4} J'_S \right) \frac{\hat{N}(\hat{N} - 1)}{2} + J'_S \cdot \hat{\mathbf{S}}_+ \cdot \hat{\mathbf{S}}_- - \left(J'_D - \frac{1}{4} J'_S \right) \sum_l \hat{N}_{l\uparrow} \hat{N}_{l\downarrow} \quad (\text{H16})$$

where $(\epsilon'_f, U', J'_D, J'_S) = \frac{32\pi^2 \zeta_x^2}{J} (-\frac{1}{2}, 1, 1, 2)$.

The two-particle eigenstates of $H_{\text{int}}^{(S)}$ are the singlet, doublet and triplet states, same as Table II except that they are formed by $\psi(0)$ -particles. They have energies

$$(E_S, E_D, E_T) = \frac{32\pi^2 \zeta_x^2}{J} (-2, -1, 0) = 2\epsilon'_f + \frac{32\pi^2 \zeta_x^2}{J} (-1, 0, 1). \quad (\text{H17})$$

The singlet state has the lowest energy, which is also less than twice the single-particle energy. Therefore, the interaction is attractive in this channel.

AD phase—In this phase, the degenerate doublet $|2\rangle, |\bar{2}\rangle$ always remains in Hilbert space, and we cannot integrate out the impurity. To see the effective interaction, we diagonalize the part of the pair-Kondo Hamiltonian that contains only the impurity and $\psi(0)$. The remaining part only adds kinetic energy to the electrons but does not affect the interaction. We start with the bosonization Hamiltonian Eq. (B35) near the fixed point and reverse all the gauge transformation and bosonization procedure to the original fermion form Eq. (B26). Notice that ψ in Eq. (B26) now is not the same as the original ψ . During RG ρ_z flows, and the gauge transformation to absorb $\rho_z \Lambda_z \partial_x \phi_v(x)|_{x=0}$ before RG uses bare ρ_z , but the inverse gauge transformation to rewrite the Hamiltonian in original form after RG uses the renormalized ρ_z .

According to Eq. (B26), the impurity and impurity-bath coupling part of the pair-Kondo Hamiltonian is

$$2\pi\lambda_z \cdot \Lambda_z \sum_{ls} l \cdot \psi_{ls}^\dagger(0) \psi_{ls}(0) + (2\pi)^2 x_c \lambda_x \left(\Lambda_+ \cdot \psi_{-\downarrow}^\dagger(0) \psi_{-\uparrow}^\dagger(0) \psi_{+\uparrow}(0) \psi_{+\downarrow}(0) + h.c. \right). \quad (\text{H18})$$

where λ_x takes the renormalized value and λ_z is related to the renormalized ρ_z by Eq. (B30). The eigenstates and energies are shown in Table VI, where we denote $\psi_{ls} \equiv \psi_{ls}(0)$ for simplicity. Notice that we have used $\delta(0) = \frac{1}{\pi x_c}$, as defined in Eq. (A17). The lowest two-particle state also has an energy less than twice the single-particle energy, indicating an attractive interaction.

To close this subsection, we add two remarks. First, the transverse couplings (ζ_x in the LS phase and λ_x in the AD phase) flow to zero only at asymptotically low energies but remain finite at intermediate scales. While they eventually vanish in the single-impurity model, in the lattice model, they may trigger pairing instabilities before vanishing through the attractive interaction they mediate. Second, the ψ electron in the Kondo-type model also contains components of the original f electron in the Anderson model, as discussed in Sec. G1. Consequently, if superconductivity could arise in the LS/AD phases due to the effective attraction acting on the ψ electron derived in this section, the pairing would involve both c - and f -electrons.

N_ψ	$[L, S]$	DEG $_{[L,S]}$	wave-function	$E \cdot x_c$
0	$[2, 0]$	2	$ 2\rangle, \bar{2}\rangle$	0
1	$[1, \frac{1}{2}]$	4	$\psi_{-s}^\dagger 2\rangle, \psi_{+s}^\dagger \bar{2}\rangle, \forall s$	$-2\lambda_z$
	$[3, \frac{1}{2}]$	4	$\psi_{+s}^\dagger 2\rangle, \psi_{-s}^\dagger \bar{2}\rangle, \forall s$	$2\lambda_z$
2	$[A_1, 0]$	1	$\frac{1}{\sqrt{2}}(\psi_{-\uparrow}^\dagger \psi_{-\uparrow}^\dagger 2\rangle - \psi_{+\uparrow}^\dagger \psi_{+\uparrow}^\dagger \bar{2}\rangle)$	$-4\lambda_z - 4\lambda_x$
	$[A_2, 0]$	1	$\frac{1}{\sqrt{2}}(\psi_{-\uparrow}^\dagger \psi_{-\uparrow}^\dagger 2\rangle + \psi_{+\uparrow}^\dagger \psi_{+\uparrow}^\dagger \bar{2}\rangle)$	$-4\lambda_z + 4\lambda_x$
	$[2, 0] \oplus [2, 1]$	8	$\psi_{+s}^\dagger \psi_{-s'}^\dagger L^z\rangle, \forall s, s', L^z$	0
	$[4, 0]$	2	$\psi_{+\uparrow}^\dagger \psi_{+\downarrow}^\dagger 2\rangle, \psi_{-\uparrow}^\dagger \psi_{-\downarrow}^\dagger \bar{2}\rangle$	$4\lambda_z$
3	$[1, \frac{1}{2}]$	4	$\psi_{+s}^\dagger \psi_{-\uparrow}^\dagger \psi_{-\downarrow}^\dagger 2\rangle, \psi_{-s}^\dagger \psi_{+\uparrow}^\dagger \psi_{+\downarrow}^\dagger \bar{2}\rangle, \forall s$	$-2\lambda_z$
	$[3, \frac{1}{2}]$	4	$\psi_{-s}^\dagger \psi_{+\uparrow}^\dagger \psi_{+\downarrow}^\dagger 2\rangle, \psi_{+s}^\dagger \psi_{-\uparrow}^\dagger \psi_{-\downarrow}^\dagger \bar{2}\rangle, \forall s$	$2\lambda_z$
4	$[2, 0]$	2	$\psi_{+\uparrow}^\dagger \psi_{+\downarrow}^\dagger \psi_{-\uparrow}^\dagger \psi_{-\downarrow}^\dagger 2\rangle, \psi_{+\uparrow}^\dagger \psi_{+\downarrow}^\dagger \psi_{-\uparrow}^\dagger \psi_{-\downarrow}^\dagger \bar{2}\rangle$	0

TABLE VI. The eigenstates of the pair-Kondo model without kinetic energy term.

I. Further details of NRG

1. Phases

Here, we describe how we distinguish the three phases by the fixed-point spectra and the spectral functions to obtain the phase diagram in the main text and End Matter.

In the FL and LS phases, the NRG spectra converge to Fermi-liquid-like fixed points. The difference between these two phases is that the ground state is non-degenerate at odd iterations in the FL phase and at even iterations in the LS phase. This is because in the FL phase, impurity electrons can hybridize with the bath electrons, whereas in the LS phase, they form a singlet and are effectively decoupled. In the AD phase, the NRG spectra converge to a family of fixed-point spectra that can be interpreted as the paired Kondo model with $\lambda_x = 0$ and different effective λ_z . We will construct effective Hamiltonians to capture these fixed-point spectra and perturbations around them in the next section. We notice that near the critical point of the FL-to-LS transition, there is an unstable fixed point (around $N = 20$ in Fig. 11 (a)(b)(d)(e) where N is the number of the iteration steps), which is consistent with the results in Ref. [115, 116]. In contrast, in the FL-to-AD transition, no new type of fixed point occurs near the critical point, as expected from the RG analysis, which shows that the critical point of the pair-Kondo model lies at the end of the fixed line.

We also plot the spectral density in Fig. 11 (g)-(i), where a sharp resonance peak, a full gap, or a dip that does not touch zero appears at zero frequency in the FL, LS, and AD phases, respectively, thereby further characterizing the three phases.

2. Effective interactions

As the RG steps increase, the NRG spectrum converges to a fixed point. Once the spectrum is close to this point, an effective Hamiltonian can be constructed by adding perturbative terms to the fixed-point Hamiltonian, thereby reproducing the small deviations of the low-energy spectrum [135, 144]. This yields an estimate of the effective interactions.

FL phase—In this phase, the fixed-point Hamiltonian is a free-fermion chain, and the leading-order correction terms are interactions at the first few sites [93, 135]. In the original NRG paper [135], Wilson *et al.* showed that the impurity site and the first bath site form a Kondo singlet and decouple from the rest of the bath. The effective Hamiltonian can then be the bath Hamiltonian without the first bath site, together with an interaction acting on the second bath site. Alternatively, Hewson *et al.* [93] proposed another effective Hamiltonian consisting of the original bath Hamiltonian and renormalized impurity interactions and impurity-bath hybridizations. Hewson's method provides an estimate of the renormalized interaction $z^2\Gamma$ and the quasiparticle weight [91, 92], which we prefer here.

Detailedly speaking, in NRG, the bath electrons are mapped to the Wilson chain, which is a free fermion chain with exponentially decaying energy scales [135, 144]

$$H^{(N)} = H_{\text{imp}} + \sum_{ls} (t_0 f_{ls}^\dagger \psi_{1ls} + h.c.) + H_{\text{bath}}^{(N)} \quad (11)$$

$$H_{\text{bath}}^{(N)} = \sum_{n=1}^N \epsilon_n \psi_{nls}^\dagger \psi_{nls} + \sum_{n=1}^{N-1} \left(t_n \psi_{nls}^\dagger \psi_{n+1ls} + h.c. \right) \quad (12)$$

where $t_N \propto \Lambda^{-\frac{N-1}{2}}$ decides the energy scale at iteration N and Λ is the discretization parameter. The H_{imp} we used is Eq. (B7). The transformation from $\Lambda^{\frac{N-1}{2}} H_N$ to $\Lambda^{\frac{N}{2}} H_{N+1}$ defines an RG transformation and the low-energy spectrum of $\Lambda^{\frac{N-1}{2}} H_N$ converges when $N \rightarrow \infty$, clarifying the fixed point.

Within T_K , the low-energy physics exhibits a Fermi-liquid feature and the effective degree of freedom is the quasiparticle $\tilde{f} \approx z^{-\frac{1}{2}} f$. Correspondingly, the low-energy NRG spectrum can be fitted by a weakly interacting model with renormalized parameters:

$$H^{(N)} = \tilde{H}_{\text{imp}} + \sum_{ls} (\tilde{t}_0 \tilde{f}_{ls}^\dagger \psi_{1ls} + h.c.) + H_{\text{bath}}^{(N)} \quad (13)$$

where $\tilde{t}_0 = z^{1/2} t_0$ and $\tilde{H}_{\text{imp}}$ takes the same form as H_{imp} except that the parameters ϵ, U, J_D, J_S are replaced by the effective values $\tilde{\epsilon}, \tilde{U}, \tilde{J}_D, \tilde{J}_S$. They are all symmetry-allowed terms in the impurity up to two-body interactions.

To obtain the renormalized parameters, we first adjust $\tilde{t}_0, \tilde{\epsilon}$ to fit the single-particle/single-hole excitation energy of H^N , by which z is also obtained. z can be alternatively obtained from the self-energy via its definition, but this approach has the drawback that the calculated self-energy depends on the chosen broadening parameters. In contrast, here z is determined solely by the NRG spectrum.

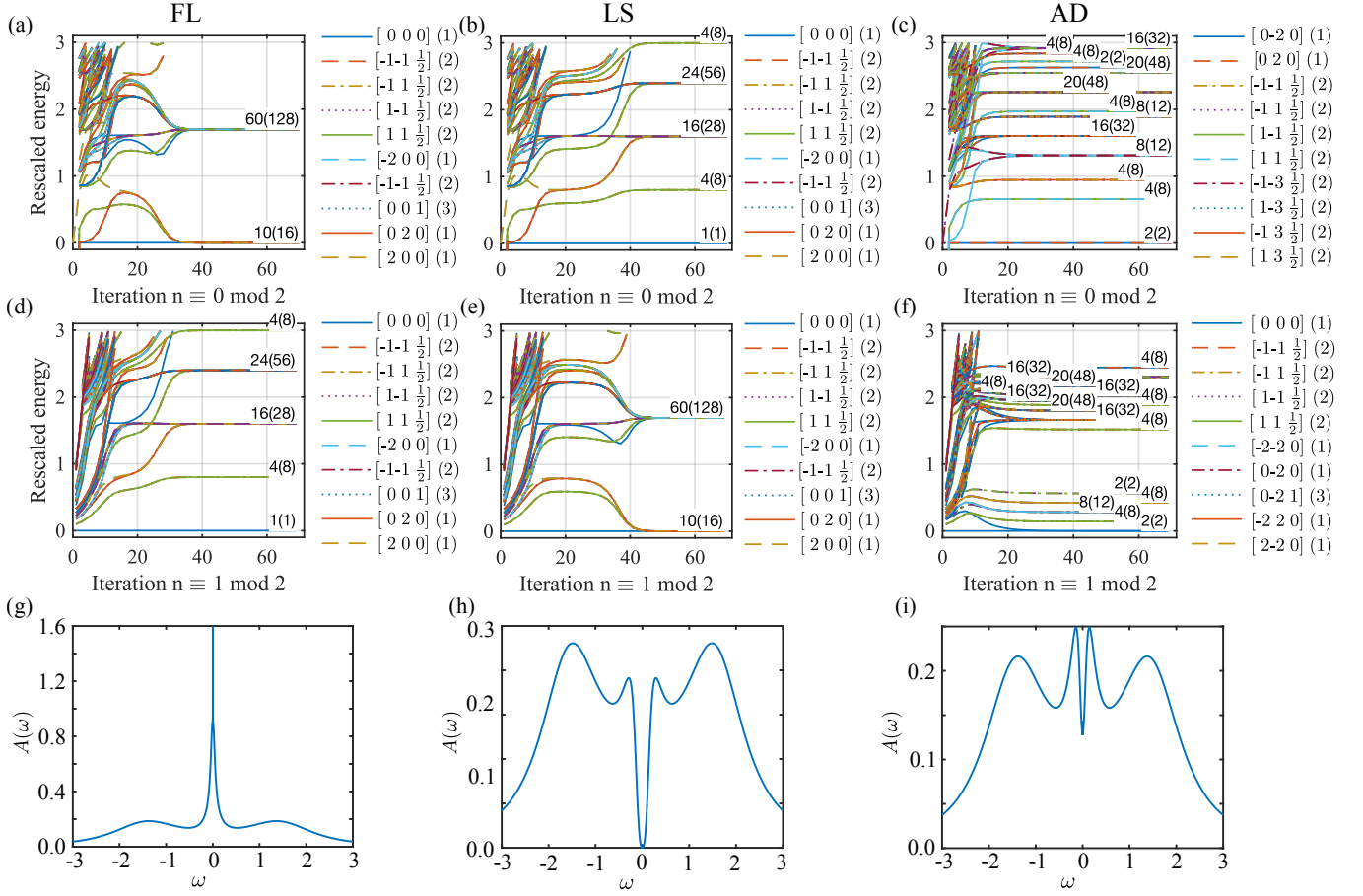


FIG. 11. Typical NRG spectrum and spectral density in three phases. Top and middle panels: NRG spectrum for even and odd numbers of bath sites, respectively. Bottom panel: The spectral density. From left to right are figures for the FL phase, the LS phase, and the AD phase. The numbers $N_{mul}(N_{state})$ next to the line indicate that the line contains N_{mul} multiplets and N_{state} states in total. $[N, L_z, S](D)$ labels the quantum number of the multiplets where N are the total particle numbers relative to half-filling, L_z is the angular momentum, S is the total spin and D is the degeneracy. We do not utilize the Z_2 valley symmetry in numerical calculations, so $\pm L_z$ are labeled differently, but one can find that the Z_2 -related states are degenerate. The parameters are chosen as follows: $J_S = 0.054$, $J_D = 0$ in the FL phase; $J_S = 0.0548$, $J_D = 0$ for the NRG spectrum, and $J_S = 0.2$, $J_D = 0$ for the spectral density in the LS phase; $J_S = 0$, $J_D = 0.2$ in the AD phase. For the local singlet phase, we use two different J_S . We choose a smaller J_S when plotting NRG spectrum so that J_S is closer to the critical point and we can illustrate the unstable fixed point in the first few iterations. We use a larger J_S when plotting spectral density because though spectral density always has a full gap but the gap shrinks when approaching the critical point.

To further obtain $\tilde{U}$, $\tilde{J}_D$, $\tilde{J}_S$, we calculate their first-order corrections to the spectrum by perturbation theory, and then match the perturbed spectrum with the one obtained by NRG. Here, we take the case where the number of bath sites is odd (i.e., the total number of sites is even) as an example. In this case, the bilinear part of the Hamiltonian can be diagonalized by

$$H_{\text{fixed}}^{(N)} = \Lambda^{-\frac{N-1}{2}} \sum_{j=1}^{\frac{N+1}{2}} \sum_{ls} \left(E_j^{(p)} c_{jls}^{(p)\dagger} c_{jls}^{(p)} - E_j^{(h)} c_{jls}^{(h)\dagger} c_{jls}^{(h)} \right) \quad (14)$$

where

- $c_{jls}^{(p)\dagger} = \alpha_{0j}^{(p)} \cdot f_{ls}^\dagger + \sum_{i=1}^N \alpha_{ij}^{(p)} \psi_{ils}^\dagger$, $c_{jls}^{(h)\dagger} = \alpha_{0j}^{(h)} \cdot f_{ls}^\dagger + \sum_{i=1}^N \alpha_{ij}^{(h)} \psi_{ils}^\dagger$ are the single-particle and single-hole eigenstates. Due to the exponentially decaying energy scale $|\alpha_{01}| \sim \Lambda^{-\frac{N}{4}}$.
- $E_1^{(p)} < E_2^{(p)} < \dots < E_{\frac{N+1}{2}}^{(p)}$ and $E_1^{(h)} < E_2^{(h)} < \dots < E_{\frac{N+1}{2}}^{(h)}$ are the single-particle/hole eigenenergies of the rescaled Hamiltonian $\Lambda^{\frac{N-1}{2}} H_{\text{fixed}}^{(N)}$, which converge to an order 1 value for fixed j and $N \rightarrow \infty$. In particle-hole symmetric case $E_j^{(p)} = E_j^{(h)}$.

We focus on the lowest single-particle state c_{1ls} and the corresponding two-particle states. To first-order perturbation, $\tilde{U}, \tilde{J}_D, \tilde{J}_S$ leave the single-particle levels unchanged. The two particle states form S, D, T multiplets, the same as those in Table II, and the eigenenergies $E_{S,D,T}$ satisfy

$$\begin{aligned} E_S - 2E_1^{(p)} &= \Lambda^{\frac{N-1}{2}} \cdot |\alpha_{01}|^4 \cdot (\tilde{U} - \tilde{J}_S) \\ E_D - 2E_1^{(p)} &= \Lambda^{\frac{N-1}{2}} \cdot |\alpha_{01}|^4 \cdot (\tilde{U} - \tilde{J}_D) \\ E_T - 2E_1^{(p)} &= \Lambda^{\frac{N-1}{2}} \cdot |\alpha_{01}|^4 \cdot \tilde{U}. \end{aligned} \quad (15)$$

We can identify the single-particle states and S, D, T multiplets by their corresponding quantum numbers in the NRG spectrum and then obtain the eigenenergies. Numerically, one will find that the left-hand sides of Eq. (15) scale as $\Lambda^{-\frac{N}{2}}$ for large enough N , and $\Lambda^{\frac{N-1}{2}} |\alpha_{01}|^4$ on the right-hand side scales as $\Lambda^{-\frac{N}{2}}$ as $|\alpha_{01}| \sim \Lambda^{-\frac{N}{4}}$, leading to finite values of $\tilde{U}, \tilde{J}_D, \tilde{J}_S$ for large N .

We plot the renormalized two-particle energies calculated from the obtained $\tilde{U}, \tilde{J}_S, \tilde{J}_D$ in Fig. 4(b-d) in the End Matter, which are consistent with the Ward identities in Sec. H1 and exhibit regions with local attractive interactions, supporting Fig. 1(b) in the main text. To further illustrate the consistency with the Ward identities, several line cuts of the renormalized parameters are shown in Fig. 4(e-g) in the End Matter.

In contrast to the works using Wilson's definition of effective interaction, which find them diverging near the critical point like Ref. [115], the effective interactions here tend to zero together with T_K , similar to Refs. [91, 94, 111]. The difference arises because Hewson's definition corresponds to the quasiparticle vertices $z^2\Gamma$, whereas Wilson's does not involve adjusting the hopping and therefore produces the bare vertices Γ , without the z^2 factor.

LS phase—Here, the fixed point is also a Fermi liquid, but the f -electron now has zero quasiparticle weight. The impurity itself forms a singlet and is decoupled from the bath; therefore, we treat the first bath as the impurity and repeat Hewson's procedure mentioned above again. In this case, we obtain the effective interaction and quasiparticle weight for the first bath site. Notably, its bare hybridization function, which will be used to fit quasiparticle z , is obtained by integrating out the other bath sites, different from the one for the impurity site that is obtained by integrating out all bath sites. As shown in Fig. 4(f) in the End Matter, with this definition, the effective parameters obtained still satisfy the prediction of Ward identities near the critical point, implying that the spin and valley moments of the first bath site are also quenched here. Ref. [111] has verified the ratio $\tilde{J}_S/\tilde{U}$ (our definition of $\tilde{J}_S$ is twice theirs). We highlight that we further find the correct definition of $\tilde{\Delta}_0$ in the LS phase and confirm that $\tilde{J}_S/\tilde{\Delta}_0, \tilde{J}_D/\tilde{\Delta}_0$ and $\tilde{U}/\tilde{\Delta}_0$ are also consistent with the Ward identities.

AD phase—For simplicity, we consider $J_S = 0$ here. Consistent with the RG analysis of the pair-Kondo model, the fixed-point Hamiltonian in the AD phase is

$$H_{\text{fixed}}^{(N)} = \tilde{\lambda}_z \Lambda_z \cdot \sum_{ls} l \psi_{1ls}^\dagger \psi_{1ls} + H_{\text{bath}}^{(N)} \quad (16)$$

where the f -impurity is left with two states $|2\rangle, |\bar{2}\rangle$ with $L_z = \pm 2$ (also $\Lambda_z = \pm 1$). The spectrum consists of two groups of free-fermion spectra. We consider even bath sites for simplicity here, which have a non-degenerate ground state before being coupled to the local moment. As Eq. (16) commutes with Λ_z , it can be diagonalized within each $\Lambda_z = \pm 1$ sector, where it is reduced to a free-fermion Hamiltonian. We then obtain

$$H_{\text{fixed}}^{(N)} = \Lambda^{-\frac{N-1}{2}} \sum_{j=1}^{N/2} \sum_{ls} \left[\left(E_j^{(p)} c_{jls}^{(p)\dagger} c_{jls}^{(p)} - E_j^{(h)} c_{jls}^{(h)\dagger} c_{jls}^{(h)} \right) + \Lambda_z \cdot l \cdot \left(\lambda_{z,j}^{(p)} c_{jls}^{(p)\dagger} c_{jls}^{(p)} + \lambda_{z,j}^{(h)} c_{jls}^{(h)\dagger} c_{jls}^{(h)} \right) \right]. \quad (17)$$

Now $c_{jls}^{(p)\dagger} = \sum_{i=1}^N \alpha_{ij}^{(p)} \psi_{ils}^\dagger$, $c_{jls}^{(h)\dagger} = \sum_{i=1}^N \alpha_{ij}^{(h)} \psi_{ils}^\dagger$. $E_j^{(p)} \pm 2\lambda_{z,j}^{(p)}$, $(E_j^{(h)} \pm 2\lambda_{z,j}^{(h)})$ are single-particle/single-hole eigenenergies of the rescaled Hamiltonian $\Lambda^{\frac{N-1}{2}} H_N$, where $+$ ($-$) corresponds to those states with bath valley charge of same (opposite) sign with the impurity. Also, $E_j^{(p)} = E_j^{(h)}$, $\lambda_{z,j}^{(p)} = \lambda_{z,j}^{(h)}$ in particle-hole symmetric case. Besides, $E_j^{(p,h)} > 2\lambda_{z,j}^{(p,h)}$, and the ground states are two-fold degenerate states $|\text{GS}\rangle_2 \equiv |2\rangle \otimes |\text{GS}\rangle_0$, $|\text{GS}\rangle_{\bar{2}} \equiv |\bar{2}\rangle \otimes |\text{GS}\rangle_0$ where $|\text{GS}\rangle_0 = \prod_{jls} c_{jls}^{(h)\dagger} |\text{vac}\rangle$ is the filled fermi sea of bath electrons.

Following Wilson [135, 144], the leading correction terms are symmetric-allowed interaction terms on the first few bath sites, and we find that the following term can account for the deviation of the NRG spectrum from the fixed point:

$$\tilde{\lambda}_x \left(\Lambda_+ \cdot \psi_{1,-\downarrow}^\dagger \psi_{1,-\uparrow}^\dagger \psi_{1+\uparrow} \psi_{1+\downarrow} + h.c. \right) \quad (18)$$

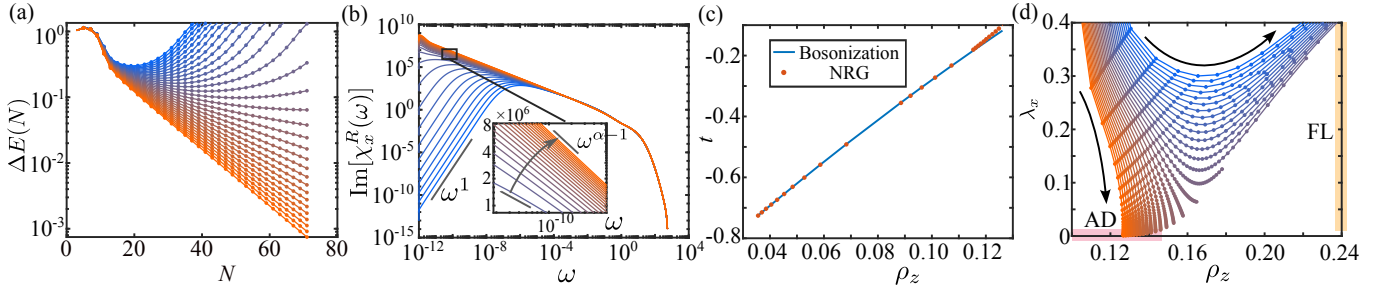


FIG. 12. NRG results near the BKT critical point. We fix $J_S = 0$ and the colors in (a),(b),(d) represent the J_D , ranging from 0.12 to 0.15 every 0.01 from blue to orange. The BKT critical point is at $J_D^{(c)} \approx 0.137$. (a) The binding energy $\Delta E(N)$ in NRG as a function of iteration step N , which corresponds to renormalized $\lambda_x(l)$ at energy scale $e^{-l} \sim \Lambda^{-N/2}$. Only even numbers of bath sites are shown. (b) Log-log plot of the imaginary part of transverse valley susceptibility $\text{Im}[\chi_x^R(\omega)]$ as a function of frequency ω near the BKT critical point. The inset shows a magnified view of the boxed region, revealing the non-universal power-law behavior $\omega^{\alpha-1}$ with $0 < \alpha < 1$ in the AD region. For those parameters in the Fermi liquid regime, $\text{Im}[\chi_x^R(\omega)] \propto \omega$ below the Kondo temperature. (c) The power t extracted from the NRG spectrum versus ρ_z extracted from the correlation function, compared with the bosonization result $t = -1 + 8\rho_z - 8\rho_z^2$. (d) RG flow of λ_x, ρ_z extracted from NRG spectrum. Each line represents λ_x, ρ_z obtained in fixed parameters and different NRG iterations. The arrow indicates the direction of RG flow when the NRG iteration step increases. Here ρ_z is calculated from λ_z .

We still focus on the single and two particle states of $c_{1ls}^{(p)}$, and drop the band index 1 hereafter for simplicity. The single particle states are also not affected by $\tilde{\lambda}_x$, while the two particle states are

$$\begin{aligned}
 & c_{+s}^\dagger c_{-s'}^\dagger |\text{GS}\rangle_{L^z, L^z = \pm 2, s = \uparrow\downarrow, s' = \uparrow\downarrow}, & E &= 2E^{(p)} \\
 & c_{+\uparrow}^\dagger c_{+\downarrow}^\dagger |\text{GS}\rangle_2, |\bar{2}\rangle \otimes c_{-\uparrow}^\dagger c_{-\downarrow}^\dagger |\text{GS}\rangle_{\bar{2}} & E &= 2E^{(p)} + 4\lambda_z^{(p)} \\
 & \frac{1}{\sqrt{2}} \left(c_{-\uparrow}^\dagger c_{-\downarrow}^\dagger |\text{GS}\rangle_2 - c_{+\uparrow}^\dagger c_{+\downarrow}^\dagger |\text{GS}\rangle_{\bar{2}} \right) & E &= 2E^{(p)} - 4\lambda_z^{(p)} - \Lambda^{(N-1)/2} \cdot |\alpha_{11}^{(p)}|^4 \cdot \tilde{\lambda}_x \\
 & \frac{1}{\sqrt{2}} \left(c_{-\uparrow}^\dagger c_{-\downarrow}^\dagger |\text{GS}\rangle_2 + c_{+\uparrow}^\dagger c_{+\downarrow}^\dagger |\text{GS}\rangle_{\bar{2}} \right) & E &= 2E^{(p)} - 4\lambda_z^{(p)} + \Lambda^{(N-1)/2} \cdot |\alpha_{11}^{(p)}|^4 \cdot \tilde{\lambda}_x.
 \end{aligned} \tag{19}$$

$|\alpha_{11}^{(p)}|$ here also decays as $\Lambda^{-N/4}$ as N increases. Unlike the cases in Fermi liquid fixed points, $\tilde{\lambda}_x$ does not converge to a fixed value when $N \rightarrow \infty$. To proceed, we define the binding energy $\Delta E(N) = 2E_p - E_{2p} \sim \Lambda^{-N/2} \tilde{\lambda}_x$ where E_p, E_{2p} are the rescaled lowest single- and two-particle energies at iteration N . Indeed, since both $\Delta E(N)$ in NRG and the running coupling $\lambda_x(l)$ in RG are rescaled under the RG flow, it is $\Delta E(N)$ instead of $\tilde{\lambda}_x$ that corresponds to λ_x in the analytical RG calculation. We identify $\lambda_x(l) = \Delta E(N)$ with $e^{-l} \sim \Lambda^{-N/2}$. As shown in Fig. 12(a), for those parameters in the AD phase, $\Delta E(N)$ shows a non-universal power law behavior $\Delta E(N) \sim \Lambda^{-tN/2}$, $0 < t < 1$, which agrees with the analytical RG analysis that $\lambda_x \sim e^{-tl}$ near the critical point (Eq. (D34)) in Sec. D.

To further elucidate this, we also numerically evaluate ρ_z and compare the obtained (t, ρ_z) to the bosonization prediction $t = -1 + 8\rho_z - 8\rho_z^2$. We plot the correlation function $\text{Im}[\chi_x^R(\omega)]$ as shown in Fig. 12(b), which shows an ordinary linear in ω dependence in the FL regime and a non-universal power law $\sim |\omega|^{\alpha-1} \text{sgn}(\omega)$ where $\alpha = 16\rho_z^2$ as proposed by Eq. (C18). We extract ρ_z from this, and t from the scaling of $\Delta E(N)$. As shown in Fig. 12(c), the relation between t and ρ_z agrees well with the bosonization prediction.

We also plot the extracted λ_x, ρ_z at each iteration in Fig. 12(d), which forms a renormalization flow as the iteration step increases. To obtain ρ_z in each iteration step, we compute it using $\rho_z = \arctan(\pi\lambda_z^{(p)})/\pi$ (Eq. (B30)) where $\lambda_z^{(p)}$ at iteration N is regarded as the renormalized λ_z at this scale. When N increases, this ρ_z converges to a fixed value which is approximately equal to the one obtained by fitting the low-energy power-law behavior of $\text{Im}[\chi_x^R(\omega)]$ mentioned above. Fig. 12(d) qualitatively reproduces the analytical RG flow from bosonization as shown in Fig. 7. Notably, the BKT critical point is close to the analytical value $\rho_z^c = \frac{1}{2} - \frac{1}{2\sqrt{2}} \approx 0.1464$.

One last concern is whether other interaction terms, such as $\tilde{U}, \tilde{J}_S, \tilde{J}_D$, will also affect the low-energy spectrum. They also contain four fermi creation/annihilation operators, and the effects on the low-energy spectrum are scaled by $\Lambda^{(N-1)/2} \cdot |\alpha_{11}^{(p)}|^4$, similar to that of $\tilde{\lambda}_x$. However, numerically, we find that the splittings due to these interaction terms are negligible compared to those of $\tilde{\lambda}_x$.