

Two channel Kondo Creutz

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A introduction

2CK has much physics ,like overscreening , non-fermi-liquid behavior , residual impurity entropy and channel symmetry. Unfortunately , few exists in flat band 2CK models , due to the system has no dispersion. Traditional methods ,like RG and bosonization can't work because all state gather within the same energy that can't be cutoff . Nevertheless , system become much simpler due to flat band and geometric effect becomes dominant.

Two major inspiration of this work is Grant Z.X. Yang Quantum Geometric Kondo Cloud and work on stub lattice. The former reveals the kondo singlet becomes kondo cloud(pure singlet) in flat band that can be controlled by quantum metric , the latter emphasize gap within flat band models can be controlled by QM that create different scaling of Superfluid weight to QM.

To realize a 2CK flat band model ,we should find a non-interacting basis that is a flat band. The cruetz ladder is just that , and its two orbitals fit the 2CK model. Moreover , we want to tune the quantum metric ,so we introduce a α term in the model that keeps flat band.

In this work , we :

- Find the kondo cloud that has 3/2 scaling law to QM due to Gap QM , more scaling also can exist in this model.
- Reveal the phase diagram of this model ,consists of a (2,2) and a (1,3) phase . Kondo singlet can have or don't have any correlation with other bath within the two phases.

B Model

We consider a spinful Creutz ladder with a localized spin-1/2 impurity. Each unit cell contains two orbitals, denoted by A and B . The Hamiltonian reads

$$H = H_0 + H_K, \tag{1}$$

where the noninteracting bath is described by

$$\begin{aligned} H_0 = & -t \sum_{j,\sigma} \left(a_{j\sigma}^\dagger b_{j+1,\sigma} + b_{j\sigma}^\dagger a_{j+1,\sigma} + \text{H.c.} \right) \\ & + t \sum_{j,\sigma} \left(-i a_{j\sigma}^\dagger a_{j+1,\sigma} + i b_{j\sigma}^\dagger b_{j+1,\sigma} + \text{H.c.} \right) \\ & + \alpha t \sum_{j,\sigma} \left(-i a_{j\sigma}^\dagger b_{j\sigma} + \text{H.c.} \right). \end{aligned} \tag{2}$$

Here, $t > 0$ sets the hopping energy scale, and α is a dimensionless intracell hopping parameter. Periodic boundary conditions are imposed.

The impurity couples symmetrically to both orbitals in unit cell j_0 :

$$H_K = J \mathbf{S}_d \cdot (\mathbf{s}_{j_0 A} + \mathbf{s}_{j_0 B}), \quad J > 0, \quad (3)$$

where

$$\mathbf{s}_{j\mu} = \frac{1}{2} \sum_{\sigma, \sigma'} c_{j\mu\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{j\mu\sigma'}, \quad \mu = A, B, \quad (4)$$

with $c_{jA\sigma} = a_{j\sigma}$ and $c_{jB\sigma} = b_{j\sigma}$. The bath electrons have no additional interaction.

We introduce the Fourier transform

$$c_{j\mu\sigma} = \frac{1}{\sqrt{L}} \sum_k e^{ikja} c_{k\mu\sigma}, \quad \mu = A, B, \quad (5)$$

where a is the lattice constant. In the orbital basis $\Psi_{k\sigma} = (a_{k\sigma}, b_{k\sigma})^T$, the bath Hamiltonian becomes

$$H_0 = \sum_{k, \sigma} \Psi_{k\sigma}^\dagger h_\alpha(k) \Psi_{k\sigma}, \quad (6)$$

with

$$\begin{aligned} h_\alpha(k) &= t \begin{pmatrix} 2 \sin(ka) & -2 \cos(ka) - i\alpha \\ -2 \cos(ka) + i\alpha & -2 \sin(ka) \end{pmatrix} \\ &= t [-2 \cos(ka) \tau_x + \alpha \tau_y + 2 \sin(ka) \tau_z], \end{aligned} \quad (7)$$

where τ_i are Pauli matrices in orbital space.

Using $\{\tau_i, \tau_j\} = 2\delta_{ij}\mathbb{I}_2$, we obtain

$$h_\alpha^2(k) = t^2 [4 \cos^2(ka) + \alpha^2 + 4 \sin^2(ka)] \mathbb{I}_2 = t^2 (4 + \alpha^2) \mathbb{I}_2. \quad (8)$$

The two spin-degenerate bands therefore have energies

$$E_\pm(k) = \pm t \sqrt{4 + \alpha^2}, \quad (9)$$

which are independent of momentum for any α . The interband gap is

$$\Delta_\alpha = 2t \sqrt{4 + \alpha^2}. \quad (10)$$

Although the energies are dispersionless, the orbital eigenstates depend on momentum. For either band and a fixed spin, the quantum metric is

$$g_\pm(k) = \text{Re} [\langle \partial_k u_\pm(k) | (\mathbb{I}_2 - |u_\pm(k)\rangle \langle u_\pm(k)|) | \partial_k u_\pm(k) \rangle]. \quad (11)$$

To evaluate it without choosing an eigenstate gauge, we introduce the band projectors

$$P_\pm(k) = \frac{1}{2} [\mathbb{I}_2 \pm \hat{\mathbf{d}}_\alpha(k) \cdot \boldsymbol{\tau}], \quad \hat{\mathbf{d}}_\alpha(k) = \frac{(-2 \cos(ka), \alpha, 2 \sin(ka))}{\sqrt{4 + \alpha^2}}. \quad (12)$$

The metric can then be expressed as

$$g_\pm(k) = \frac{1}{2} \text{Tr} [(\partial_k P_\pm(k))^2] = \frac{1}{4} \left| \partial_k \hat{\mathbf{d}}_\alpha(k) \right|^2. \quad (13)$$

Since

$$\partial_k \hat{\mathbf{d}}_\alpha(k) = \frac{2a}{\sqrt{4 + \alpha^2}} (\sin(ka), 0, \cos(ka)), \quad (14)$$

both bands possess the same momentum-independent metric,

$$\boxed{g_\pm(k) = \frac{a^2}{4 + \alpha^2}}. \quad (15)$$

Consequently, its Brillouin-zone average and the associated quantum metric length are

$$\bar{g} \equiv \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk g_\pm(k) = \frac{a^2}{4 + \alpha^2}, \quad \ell_{\text{QM}} \equiv \sqrt{\bar{g}} = \frac{a}{\sqrt{4 + \alpha^2}}. \quad (16)$$

Thus, α continuously tunes the quantum metric while preserving the exact flatness of both bands.

C Small J – ‘kondo cloud’ scaling with tunable quantum metric

C.1 Weak-exchange scaling with the quantum metric

We consider half filling, $N_e = 2L$, and $J/\Delta_\alpha \ll 1$. We shift the origin to the impurity rung, $j_0 = 0$, and define $\mathbf{s}_j = \mathbf{s}_{jA} + \mathbf{s}_{jB}$.

Definition of the impurity–bath correlation. We use the full scalar spin correlation,

$$C_j = \langle \mathbf{S}_d \cdot \mathbf{s}_j \rangle, \quad C(q) = \sum_j e^{-iqx_j} C_j, \quad x_j = ja. \quad (17)$$

No product of local magnetizations is subtracted. The signed, unnormalized second moment is

$$M_2 = \sum_j x_j^2 C_j. \quad (18)$$

First-order perturbation theory for C_j . In the sector with total $S^z = 1/2$, the unperturbed state is

$$|\Psi_0\rangle = |\uparrow\rangle_d \otimes |\text{BI}\rangle. \quad (19)$$

At half filling, each lower-band Bloch orbital is occupied by both spin components, while the upper band is empty. The resulting band-insulator bath is a spin singlet, and therefore

$$\langle \text{BI} | \mathbf{s}_j | \text{BI} \rangle = 0, \quad \langle \Psi_0 | H_K | \Psi_0 \rangle = 0. \quad (20)$$

In particular, H_K has no matrix elements within the unperturbed ground-state doublet.

Acting on the filled lower band, $\mathbf{s}_0$ creates an interband particle–hole excitation. Intra-band excitations within the lower band are Pauli blocked, and the upper band contains no electrons. Because both bands are flat, every intermediate state generated in this way has the same excitation energy Δ_α .

The first-order correction to the wavefunction is therefore

$$\begin{aligned} |\Psi^{(1)}\rangle &= \sum_{n \neq 0} |n\rangle \frac{\langle n | H_K | \Psi_0 \rangle}{E_{\text{BI}} - E_n} \\ &= -\frac{J}{\Delta_\alpha} \sum_{b=x,y,z} S_d^b s_0^b | \Psi_0 \rangle. \end{aligned} \quad (21)$$

The zeroth-order contribution to C_j vanishes. Keeping the two first-order wavefunction contributions gives

$$\begin{aligned} C_j^{(1)} &= \langle \Psi_0 | \mathbf{S}_d \cdot \mathbf{s}_j | \Psi^{(1)} \rangle + \langle \Psi^{(1)} | \mathbf{S}_d \cdot \mathbf{s}_j | \Psi_0 \rangle \\ &= -\frac{2J}{\Delta_\alpha} \text{Re} \sum_{a,b} \langle S_d^a S_d^b \rangle_0 \langle s_j^a s_0^b \rangle_0. \end{aligned} \quad (22)$$

$$\langle \Psi_0 | S_d^a S_d^b s_j^a s_0^b | \Psi_0 \rangle = \langle \uparrow | S_d^a S_d^b | \uparrow \rangle \langle \text{BI} | s_j^a s_0^b | \text{BI} \rangle. \quad (23)$$

The factor of two comes from the corrections to the bra and the ket. Spin-rotation invariance of the unperturbed bath implies

$$[\langle s_j^a s_0^b \rangle_0]_{a,b=x,y,z} = \begin{pmatrix} A_j & 0 & 0 \\ 0 & A_j & 0 \\ 0 & 0 & A_j \end{pmatrix}. \quad (24)$$

$$\langle s_j^a s_0^b \rangle_0 = \delta_{ab} A_j, \quad A_j \equiv \langle s_j^z s_0^z \rangle_0. \quad (25)$$

Using

$$\sum_a \langle (S_d^a)^2 \rangle_0 = S_d(S_d + 1) = \frac{3}{4}, \quad (26)$$

$$\sum_{a,b} \langle S_d^a S_d^b \rangle_0 \langle s_j^a s_0^b \rangle_0 = \sum_{a,b} \langle S_d^a S_d^b \rangle_0 \delta_{ab} A_j \quad (27)$$

$$= A_j \sum_a \langle S_d^a S_d^a \rangle_0 \quad (28)$$

$$= A_j [\langle (S_d^x)^2 \rangle_0 + \langle (S_d^y)^2 \rangle_0 + \langle (S_d^z)^2 \rangle_0]. \quad (29)$$

we obtain

$$C_j = -\frac{3J}{2\Delta_\alpha} A_j + O[(J/\Delta_\alpha)^2]. \quad (30)$$

Thus the leading impurity–bath correlation is determined by the equal-time spin correlation of the unperturbed bath.

Fourier transformation of the bath correlation. Define

$$s_q^z = \sum_j e^{-iqja} s_j^z, \quad A(q) = \sum_j e^{-iqja} A_j. \quad (31)$$

Expanding the product of Fourier components gives

$$\langle s_q^z s_{-q}^z \rangle_0 = \sum_{j,l} e^{-iq(j-l)a} \langle s_j^z s_l^z \rangle_0. \quad (32)$$

The unperturbed bath is translationally invariant, so $\langle s_j^z s_l^z \rangle_0 = A_{j-l}$. For each relative separation $r = j - l$, there are L choices of l . Hence

$$\langle s_q^z s_{-q}^z \rangle_0 = L \sum_r e^{-iqra} A_r = LA(q). \quad (33)$$

Consequently,

$$A(q) = \frac{1}{L} \langle s_q^z s_{-q}^z \rangle_0, \quad C^{(1)}(q) = -\frac{3J}{2\Delta_\alpha L} \langle s_q^z s_{-q}^z \rangle_0. \quad (34)$$

Only the unperturbed bath is assumed to be translationally invariant; the impurity breaks translation symmetry in the interacting system.

We use the electronic Fourier convention

$$c_{j\mu\sigma} = \frac{1}{\sqrt{L}} \sum_k e^{ikja} c_{k\mu\sigma}. \quad (35)$$

Writing $\eta_\uparrow = 1$ and $\eta_\downarrow = -1$, the spin density becomes

$$\begin{aligned} s_q^z &= \frac{1}{2} \sum_{j,\mu,\sigma} e^{-iqja} \eta_\sigma c_{j\mu\sigma}^\dagger c_{j\mu\sigma} \\ &= \frac{1}{2} \sum_{k,\mu,\sigma} \eta_\sigma c_{k\mu\sigma}^\dagger c_{k+q,\mu\sigma}. \end{aligned} \quad (36)$$

The momentum constraint follows from

$$\frac{1}{L} \sum_j e^{i(k'-k-q)ja} = \delta_{k',k+q}. \quad (37)$$

Wick contraction and the band projectors. Let $P_\pm(k)$ denote the orbital projectors onto the upper and lower bands. Since the lower band is filled for both spins,

$$\langle c_{k\mu\sigma}^\dagger c_{k'\nu\sigma'} \rangle_0 = \delta_{kk'} \delta_{\sigma\sigma'} [P_-(k)]_{\nu\mu}, \quad (38)$$

$$\langle c_{k\mu\sigma} c_{k'\nu\sigma'}^\dagger \rangle_0 = \delta_{kk'} \delta_{\sigma\sigma'} [P_+(k)]_{\mu\nu}. \quad (39)$$

The second relation follows from the fermionic anticommutation relation and $I - P_- = P_+$.

Substituting Eq. (36), we find

$$\langle s_q^z s_{-q}^z \rangle_0 = \frac{1}{4} \sum_{\substack{k,p,\mu,\nu \\ \sigma,\sigma'}} \eta_\sigma \eta_{\sigma'} \langle c_{k\mu\sigma}^\dagger c_{k+q,\mu\sigma} c_{p\nu\sigma'}^\dagger c_{p-q,\nu\sigma'} \rangle_0. \quad (40)$$

For this operator ordering, Wick's theorem reads

$$\langle c_1^\dagger c_2 c_3^\dagger c_4 \rangle_0 = \langle c_1^\dagger c_2 \rangle_0 \langle c_3^\dagger c_4 \rangle_0 + \langle c_1^\dagger c_4 \rangle_0 \langle c_2 c_3^\dagger \rangle_0. \quad (41)$$

The first term yields $\langle s_q^z \rangle_0 \langle s_{-q}^z \rangle_0 = 0$. The second term imposes $p = k + q$ and $\sigma' = \sigma$, giving

$$\begin{aligned} \langle s_q^z s_{-q}^z \rangle_0 &= \frac{1}{4} \sum_{k,\mu,\nu,\sigma} \eta_\sigma^2 [P_-(k)]_{\nu\mu} [P_+(k+q)]_{\mu\nu} \\ &= \frac{1}{2} \sum_k \text{Tr}[P_-(k) P_+(k+q)]. \end{aligned} \quad (42)$$

Here $\sum_{\sigma} \eta_{\sigma}^2 = 2$, while the orbital sum produces the trace. Combining Eqs. (34) and (42), we obtain

$$C^{(1)}(q) = -\frac{3J}{4\Delta_{\alpha}L} \sum_k \text{Tr}[P_{-}(k)P_{+}(k+q)]. \quad (43)$$

Explicit evaluation for the Creutz- α bath. The band projectors are

$$P_{\pm}(k) = \frac{1}{2} [I \pm \mathbf{n}_{\alpha}(k) \cdot \boldsymbol{\tau}], \quad \mathbf{n}_{\alpha}(k) = \frac{(-2 \cos ka, \alpha, 2 \sin ka)}{\sqrt{4 + \alpha^2}}. \quad (44)$$

Using $\text{Tr} \tau_i = 0$ and $\text{Tr}(\tau_i \tau_j) = 2\delta_{ij}$,

$$\text{Tr}[P_{-}(k)P_{+}(k+q)] = \frac{1}{2} [1 - \mathbf{n}_{\alpha}(k) \cdot \mathbf{n}_{\alpha}(k+q)]. \quad (45)$$

The scalar product evaluates to

$$\begin{aligned} \mathbf{n}_{\alpha}(k) \cdot \mathbf{n}_{\alpha}(k+q) &= \frac{4 \cos(ka) \cos[(k+q)a] + 4 \sin(ka) \sin[(k+q)a] + \alpha^2}{4 + \alpha^2} \\ &= \frac{4 \cos(qa) + \alpha^2}{4 + \alpha^2}. \end{aligned} \quad (46)$$

Therefore,

$$\text{Tr}[P_{-}(k)P_{+}(k+q)] = \frac{2[1 - \cos(qa)]}{4 + \alpha^2}. \quad (47)$$

This expression is independent of k , so the momentum sum in Eq. (43) simply contributes a factor of L . We obtain

$$C^{(1)}(q) = -\frac{3J}{2\Delta_{\alpha}(4 + \alpha^2)} [1 - \cos(qa)]. \quad (48)$$

This result retains the full wave-vector dependence; only the exchange coupling has been expanded.

For either band, the quantum metric is

$$\begin{aligned} g_{\alpha}(k) &= \frac{1}{4} |\partial_k \mathbf{n}_{\alpha}(k)|^2 \\ &= \frac{1}{4} \frac{4a^2 \sin^2(ka) + 4a^2 \cos^2(ka)}{4 + \alpha^2} = \frac{a^2}{4 + \alpha^2} \equiv \bar{g}_{\alpha}. \end{aligned} \quad (49)$$

Equation (48) can thus be written as

$$C(q) = -\frac{3J}{2\Delta_{\alpha}} \frac{\bar{g}_{\alpha}}{a^2} [1 - \cos(qa)] + O[(J/\Delta_{\alpha})^2]. \quad (50)$$

Second moment and its geometric dependence. Differentiating the Fourier definition gives

$$\frac{\partial^2 C(q)}{\partial q^2} = -\sum_j x_j^2 e^{-iqx_j} C_j. \quad (51)$$

Hence

$$M_2 = - \left. \frac{\partial^2 C(q)}{\partial q^2} \right|_{q=0}. \quad (52)$$

Since

$$\left. \frac{\partial^2}{\partial q^2} [1 - \cos(qa)] \right|_{q=0} = a^2, \quad (53)$$

Eq. (50) yields

$$\boxed{M_2 = \frac{3J}{2\Delta_\alpha} \bar{g}_\alpha + O[a^2(J/\Delta_\alpha)^2]}. \quad (54)$$

Equivalently, the small- q expansion is

$$C^{(1)}(q) = -\frac{3J\bar{g}_\alpha}{4\Delta_\alpha} q^2 + O[(J/\Delta_\alpha)a^4 q^4]. \quad (55)$$

Thus M_2 measures the curvature of the impurity–bath spin correlation at zero wave vector. Because the real-space correlation retains its sign, M_2 is not a normalized spatial variance.

For a finite periodic system, the derivative is understood through the continuous function $\sum_j e^{-iqx_j} C_j$ associated with the chosen real-space coordinates. It does not require a numerical derivative of the discrete momentum data.

The 3/2 scaling at fixed t . Substituting the explicit gap into Eq. (54), the first-order result is

$$M_2^{(1)} = \frac{3Ja^2}{4t(4 + \alpha^2)^{3/2}}. \quad (56)$$

The metric and gap obey

$$\bar{g}_\alpha = \frac{a^2}{4 + \alpha^2}, \quad \sqrt{4 + \alpha^2} = \frac{a}{\sqrt{\bar{g}_\alpha}}, \quad \Delta_\alpha = \frac{2ta}{\sqrt{\bar{g}_\alpha}}. \quad (57)$$

Eliminating Δ_α gives

$$M_2^{(1)} = \frac{3J}{2} \bar{g}_\alpha \frac{\sqrt{\bar{g}_\alpha}}{2ta} = \frac{3J}{4ta} \bar{g}_\alpha^{3/2}, \quad (58)$$

$$\boxed{\frac{M_2^{(1)}}{a^2} = \frac{3J}{4t} \left(\frac{\bar{g}_\alpha}{a^2} \right)^{3/2}}. \quad (59)$$

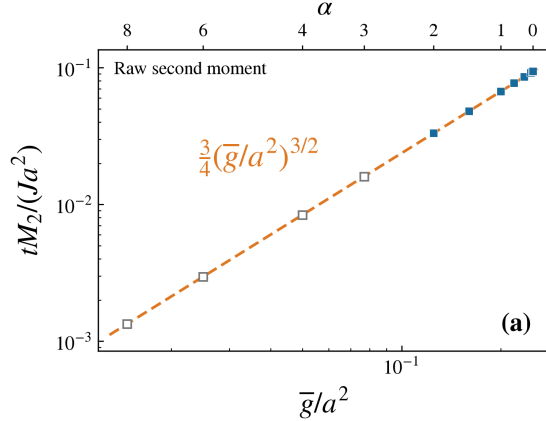
The exponent combines the geometric matrix-element factor $\bar{g}_\alpha$ with the inverse excitation gap $\Delta_\alpha^{-1} \propto \bar{g}_\alpha^{1/2}$. This relation holds at first order in J throughout the fixed- t parameter path, provided $J/\Delta_\alpha \ll 1$. In particular, its local logarithmic slope is

$$\frac{d \ln[tM_2^{(1)} / (Ja^2)]}{d \ln(\bar{g}_\alpha / a^2)} = \frac{3}{2}, \quad (60)$$

including the limit $\alpha \rightarrow 0$.

C.2 DMRG realization

We evaluate the original-lattice spin correlations at $J/t = 0.05$, $L = 32$, and $N_e = 64$ with periodic boundary conditions. The observable is $tM_2/(Ja^2)$ as a function of $\bar{g}_\alpha/a^2$ along the fixed- t path. The eight converged points in the wider parameter scan give a logarithmic slope $p = 1.5013$; four unconverged checkpoints are shown only for reference and are excluded from the fit. Five additional calculations at $\alpha = 0, 0.01, 0.02, 0.03, 0.04$ all satisfy the convergence criteria and yield a local slope $p = 1.50143$. The latter fit covers a narrow relative metric variation of approximately 0.04% and is a local slope test.



(a) Wider α range.

C.3 Spectral weights, effective excitation gaps, and geometric scaling

Consider

$$H = H_0(\eta) + \lambda V, \quad V = \frac{1}{2N} \sum_{q,a,b} v_{ab}(q) : O_a(q) O_b(-q) :, \quad O_a^\dagger(q) = O_a(-q). \quad (61)$$

Here η tunes the band structure. We assume a gapped reference ground state and a regular weak- λ expansion.

Spectral representation. For a selected operator channel O , define

$$\mathcal{S}_O(q, \omega) = \frac{1}{N} \sum_{n \neq 0} |\langle n | O(-q) | 0 \rangle|^2 \delta(\omega - \omega_n), \quad \omega_n = E_n - E_0. \quad (62)$$

Completeness gives

$$m_0(q) \equiv \int_0^\infty d\omega \mathcal{S}_O(q, \omega) = \frac{1}{N} \langle O(q) O(-q) \rangle_c. \quad (63)$$

For equal spectral weights at q and $-q$,

$$\chi_O(q) = \frac{2}{N} \sum_{n \neq 0} \frac{|\langle n | O(-q) | 0 \rangle|^2}{\omega_n} = 2 \int_0^\infty \frac{d\omega}{\omega} \mathcal{S}_O(q, \omega) \equiv 2m_{-1}(q). \quad (64)$$

Therefore,

$$\Delta_{\text{eff},O}(q) \equiv \frac{m_0(q)}{m_{-1}(q)}, \quad \chi_O(q) = \frac{2m_0(q)}{\Delta_{\text{eff},O}(q)}. \quad (65)$$

Equivalently,

$$\frac{1}{\Delta_{\text{eff},O}(q)} = \sum_{n \neq 0} \frac{w_n(q)}{\omega_n}, \quad w_n(q) = \frac{|\langle n|O(-q)|0 \rangle|^2}{\sum_{m \neq 0} |\langle m|O(-q)|0 \rangle|^2}. \quad (66)$$

Thus $\Delta_{\text{eff},O}$ is a response-weighted harmonic mean, rather than necessarily the minimum gap.

Derivation of the long-wavelength spectral density. Consider a noninteracting band insulator with one occupied orbital band, labelled 0, and empty bands labelled m . We choose an orbital-identity density vertex:

$$O(-q) = \sum_{k,\mu,s,s'} c_{k+q,\mu s'}^\dagger T_{s's} c_{k,\mu s}. \quad (67)$$

The internal components have identical band structures and occupations. Using

$$c_{k,\mu s} = \sum_n u_{\mu n}(k) \gamma_{kns}, \quad (68)$$

we obtain

$$O(-q) = \sum_{k,m,n,s,s'} T_{s's} \langle u_m(k+q) | u_n(k) \rangle \gamma_{k+q,m,s'}^\dagger \gamma_{k,n,s}. \quad (69)$$

Acting on the band-insulator ground state, the inelastic part of this operator creates one particle-hole pair:

$$|k, m; s', s; q\rangle = \gamma_{k+q,m,s'}^\dagger \gamma_{k,0,s} |\text{BI}\rangle, \quad m \neq 0. \quad (70)$$

These states are normalized and have excitation energies

$$\omega_{km}(q) = \epsilon_m(k+q) - \epsilon_0(k). \quad (71)$$

Their matrix elements follow directly from Eq. (69):

$$\langle k, m; s', s; q | O(-q) | \text{BI} \rangle = T_{s's} \langle u_m(k+q) | u_0(k) \rangle. \quad (72)$$

Substituting these matrix elements into the Lehmann representation,

$$\mathcal{S}_O(q, \omega) = \frac{1}{N} \sum_{\ell \neq 0} |\langle \ell | O(-q) | \text{BI} \rangle|^2 \delta(\omega - \omega_\ell), \quad (73)$$

gives the finite- q expression

$$\mathcal{S}_O(q, \omega) = \frac{\nu}{N} \sum_{k,m \neq 0} |\langle u_m(k+q) | u_0(k) \rangle|^2 \delta[\omega - \epsilon_m(k+q) + \epsilon_0(k)], \quad (74)$$

where

$$\nu = \sum_{s,s'} |T_{s's}|^2 = \text{Tr}(T^\dagger T). \quad (75)$$

The factor $1/N$ comes from the definition of the spectral density; the internal-state sum produces ν .

We next expand the interband overlap. Since $\langle u_m(k)|u_0(k)\rangle = 0$,

$$\begin{aligned}\langle u_m(k+q)|u_0(k)\rangle &= q\langle \partial_k u_m(k)|u_0(k)\rangle + O(q^2) \\ &= -q\langle u_m(k)|\partial_k u_0(k)\rangle + O(q^2).\end{aligned}\tag{76}$$

The second equality follows from

$$\partial_k \langle u_m(k)|u_0(k)\rangle = \langle \partial_k u_m|u_0\rangle + \langle u_m|\partial_k u_0\rangle = 0.\tag{77}$$

Therefore,

$$|\langle u_m(k+q)|u_0(k)\rangle|^2 = q^2 g_m(k) + O(q^3), \quad g_m(k) = |\langle u_m(k)|\partial_k u_0(k)\rangle|^2.\tag{78}$$

The excitation energy also depends on q :

$$\omega_{km}(q) = \Delta_m(k) + qv_m(k) + O(q^2), \quad \Delta_m(k) = \epsilon_m(k) - \epsilon_0(k), \quad v_m(k) = \partial_k \epsilon_m(k).\tag{79}$$

In the distributional sense,

$$\delta[\omega - \omega_{km}(q)] = \delta[\omega - \Delta_m(k)] - qv_m(k)\delta'[\omega - \Delta_m(k)] + O(q^2).\tag{80}$$

Since the squared matrix element already starts at q^2 , the q dependence of the excitation energy first contributes at order q^3 . Thus

$$\begin{aligned}|\langle u_m(k+q)|u_0(k)\rangle|^2 \delta[\omega - \omega_{km}(q)] \\ = q^2 g_m(k) \delta[\omega - \Delta_m(k)] + O(q^3).\end{aligned}\tag{81}$$

Substitution into Eq. (74) yields

$$\mathcal{S}_O(q, \omega) = q^2 \frac{\nu}{N} \sum_{k, m \neq 0} g_m(k) \delta[\omega - \Delta_m(k)] + O(q^3).\tag{82}$$

If the full spectral density is even in q and admits a regular expansion, the odd-order terms vanish:

$$\boxed{\mathcal{S}_O(q, \omega) = q^2 \mathcal{G}_O(\omega) + O(q^4), \quad \mathcal{G}_O(\omega) = \frac{\nu}{N} \sum_{k, m \neq 0} g_m(k) \delta[\omega - \Delta_m(k)].}\tag{83}$$

For exactly flat occupied and empty bands, the excitation energies are independent of q from the outset.

Finally, completeness of the empty-band eigenvectors gives

$$\sum_{m \neq 0} g_m(k) = \langle \partial_k u_0 | (I - |u_0\rangle\langle u_0|) | \partial_k u_0 \rangle = g(k),\tag{84}$$

$$\int_0^\infty d\omega \mathcal{G}_O(\omega) = \frac{\nu}{N} \sum_k g(k) = \nu \bar{g}.\tag{85}$$

Thus the quantum metric is the integrated leading long-wavelength spectral weight, while $\mathcal{G}_O(\omega)$ additionally resolves how that weight is distributed over excitation energies.

Consequently,

$$m_0(q) = \nu \bar{g} q^2 + O(q^4), \quad \bar{g} = \frac{1}{N} \sum_k g(k), \quad (86)$$

$$m_{-1}(q) = \frac{\nu q^2}{N} \sum_{k, m \neq 0} \frac{g_m(k)}{\Delta_m(k)} + O(q^4). \quad (87)$$

Hence

$$\Delta_{\text{eff}} = \frac{\sum_{k, m \neq 0} g_m(k)}{\sum_{k, m \neq 0} g_m(k)/\Delta_m(k)}, \quad \chi_O(q) = \frac{2\nu \bar{g}}{\Delta_{\text{eff}}} q^2 + O(q^4). \quad (88)$$

Geometry enters both the total weight and its distribution over excitation energies. For two groups of transitions,

$$\bar{g} = g_1 + g_2, \quad \Delta_{\text{eff}} = \frac{g_1 + g_2}{g_1/\Delta_1 + g_2/\Delta_2}. \quad (89)$$

Redistributing g_1, g_2 changes Δ_{eff} even at fixed $\bar{g}, \Delta_1, \Delta_2$.

Interaction-induced correlation and second moment. For an interaction channel whose first-order calculation gives

$$C(q) = -\lambda c(\eta) \chi_O(q) + O(\lambda^2), \quad (90)$$

the preceding spectral expression yields

$$C^{(1)}(q) = -\frac{2\lambda c(\eta) \nu(\eta) \bar{g}(\eta)}{\Delta_{\text{eff}}(\eta)} q^2 + O(q^4). \quad (91)$$

Using

$$C(q) = \sum_j e^{-iqx_j} C_j, \quad M_2 = \sum_j x_j^2 C_j = -C''(0), \quad (92)$$

we obtain

$$M_2^{(1)} = \lambda \mathcal{A}(\eta) \frac{\bar{g}(\eta)}{\Delta_{\text{eff}}(\eta)}, \quad \mathcal{A} = 4c\nu. \quad (93)$$

For the spin-1/2 Kondo correlation, $c = 3/4$ and $\nu = 1/2$, giving

$$M_2^{(1)} = \frac{3J}{2\Delta_{\text{eff}}} \bar{g}. \quad (94)$$

Scaling exponent. Along a monotonic parameter path, define $x = \bar{g}/g_*$, with fixed reference metric g_* . Then

$$\ln |M_2^{(1)}/\lambda| = \ln |\mathcal{A}| + \ln \bar{g} - \ln \Delta_{\text{eff}}, \quad (95)$$

$$p \equiv \frac{d \ln |M_2^{(1)}/\lambda|}{d \ln x} = 1 + \frac{d \ln |\mathcal{A}|}{d \ln x} - \frac{d \ln \Delta_{\text{eff}}}{d \ln x}. \quad (96)$$

In particular, if $\mathcal{A}$ is constant,

$$\Delta_{\text{eff}} \propto x^{-\beta} \implies M_2^{(1)} \propto \lambda x^{1+\beta}. \quad (97)$$

For the case relevant here,

$$\Delta_{\text{eff}} \propto \bar{g}^{-1/2} \implies \beta = \frac{1}{2}, \quad p = 1 + \frac{1}{2} = \frac{3}{2}. \quad (98)$$

For the fixed- t Creutz- α family,

$$\bar{g}_\alpha = \frac{a^2}{4 + \alpha^2}, \quad \Delta_\alpha = 2t\sqrt{4 + \alpha^2} = \frac{2ta}{\sqrt{\bar{g}_\alpha}}, \quad (99)$$

and therefore

$$\boxed{\frac{M_2^{(1)}}{a^2} = \frac{3J}{4t} \left(\frac{\bar{g}_\alpha}{a^2} \right)^{3/2}}. \quad (100)$$

These results require a finite reference gap. If the interaction itself generates $\Delta_{\text{eff}} \propto \lambda$ inside a degenerate flat-band manifold, the factor of λ may cancel against the denominator; ordinary nondegenerate first-order perturbation theory then does not apply.

C.4 What to do

Change the parameter to this can truly have two modes, and still flat band. [Useless]

$$t_\alpha = \sqrt{A + \frac{1}{4 + \alpha^2}}. \quad (101)$$

If $A \gg \frac{1}{4 + \alpha^2}$ is 1, If $A \ll \frac{1}{4 + \alpha^2}$ is $3/2$

Intersting, if $\Delta = g$ or even $\Delta = g^2$, then $M = \text{const}$ or $M = g^{-1}$, which means larger wannier spread, smaller kondo spin correlation. In this model We can fix $m = \alpha t$, so that $M(t)$ is function of t . t controls gap, larger t means larger gap. But M grows when $t < \sqrt{2}$, declines when $t > \sqrt{2}$. Relation of gap with kondo correlation may be intersting. Which two physics are competing here, how to observe it?

D large J Phase Digram

D.1 dimer basis

Construction of the central and outer orbitals. We want to define a complete basis for flat band electrons. Define orbital position at impurity is 0, after is 1, before is -1. $|j\mu\rangle$ is a single particle state. j is position μ is A or B. We ignore spin in non-interacting because no exchange spin here. Let

$$T = t(-\tau_x - i\tau_z), \quad \tau_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

The choice of the central rung is determined by the location of the impurity, rather than by the flat-band identity alone. For an arbitrary rung j , define the single-particle subspace

$$\mathcal{K}_j = \text{span} \{h^n |j, \mu\rangle : n = 0, 1, \dots, \mu = A, B\}. \quad (102)$$

Since $h^2 = \varepsilon^2 I$, we have

$$h^{2n} |j, \mu\rangle = \varepsilon^{2n} |j, \mu\rangle, \quad h^{2n+1} |j, \mu\rangle = \varepsilon^{2n} h |j, \mu\rangle. \quad (103)$$

Consequently, K is 'next direct' product of K_j

$$\boxed{\mathcal{K}_j = \text{span} \{ |j, A\rangle, |j, B\rangle, h|j, A\rangle, h|j, B\rangle \}, \quad \dim \mathcal{K}_j \leq 4.} \quad (104)$$

Thus, an arbitrary rung can generate such a finite-dimensional invariant subspace. These subspaces need not coincide, and none is claimed to span the entire bath.

The exchange interaction

$$H_K = J\mathbf{S}_d \cdot (\mathbf{s}_{0A} + \mathbf{s}_{0B}) \quad (105)$$

selects $\mathcal{K}_0$ as the impurity-active single-particle subspace. By construction,

$$h\mathcal{K}_0 \subseteq \mathcal{K}_0. \quad (106)$$

Hermiticity then guarantees that its orthogonal complement is also invariant: for $|\phi\rangle \in \mathcal{K}_0$ and $|\chi\rangle \in \mathcal{K}_0^\perp$,

$$\langle \phi | h | \chi \rangle = \langle h\phi | \chi \rangle = 0. \quad (107)$$

Therefore, the full single-particle bath space decomposes as

$$\boxed{\mathcal{H}_{\text{bath}}^{(1)} = \mathcal{K}_0 \oplus \mathcal{K}_0^\perp,} \quad (108)$$

with no bath hopping between the two subspaces. Moreover, $\mathcal{K}_0^\perp$ has zero overlap with the central orbitals, so the local exchange acts entirely within the Fock space generated by $\mathcal{K}_0$.

$$h = \sum_{j,\mu,\nu} \left[T_{\mu\nu} |j\mu\rangle \langle j+1, \nu| \right. \quad (109)$$

$$\left. + (T^\dagger)_{\mu\nu} |j+1, \mu\rangle \langle j\nu| \right. \quad (110)$$

$$\left. + m(\tau_y)_{\mu\nu} |j\mu\rangle \langle j\nu| \right], \quad (111)$$

$$\Pi_0 = |0A\rangle \langle 0A| + |0B\rangle \langle 0B| \quad (112)$$

project onto the impurity rung. The local bath matrix is

$$\Pi_0 h \Pi_0 = m\tau_y. \quad (113)$$

Choose its orthonormal eigenvectors

$$|c_s\rangle = \frac{|0A\rangle + is|0B\rangle}{\sqrt{2}}, \quad s = \pm 1. \quad (114)$$

They obey

$$\Pi_0 h |c_s\rangle = sm |c_s\rangle, \quad \langle c_{s'} | c_s \rangle = \delta_{s's}. \quad (115)$$

Define two additional orbitals by

$$\boxed{|d_s\rangle = \frac{(h - sm)|c_s\rangle}{v}.} \quad (116)$$

Their central components vanish:

$$\Pi_0|d_s\rangle = \frac{\Pi_0 h|c_s\rangle - sm|c_s\rangle}{v} \quad (117)$$

$$= 0. \quad (118)$$

Therefore,

$$\langle c_{s'}|d_s\rangle = 0 \quad \text{for all } s, s'. \quad (119)$$

The normalization follows from

$$\langle d_s|d_s\rangle = \frac{\langle c_s|(h - sm)^2|c_s\rangle}{v^2} \quad (120)$$

$$= \frac{\varepsilon^2 - 2sm\langle c_s|h|c_s\rangle + m^2}{v^2} \quad (121)$$

$$= \frac{\varepsilon^2 - m^2}{v^2} \quad (122)$$

$$= 1. \quad (123)$$

The two outer orbitals are also orthogonal:

$$\langle d_+|d_- \rangle = \frac{\langle c_+|(h - m)(h + m)|c_- \rangle}{v^2} \quad (124)$$

$$= \frac{\langle c_+|(h^2 - m^2)|c_- \rangle}{v^2} \quad (125)$$

$$= \frac{\varepsilon^2 - m^2}{v^2} \langle c_+|c_- \rangle \quad (126)$$

$$= 0. \quad (127)$$

Thus

$$\mathcal{H}_{\text{act}}^{(1)} = \text{span} \{|c_+\rangle, |d_+\rangle, |c_-\rangle, |d_-\rangle\} \quad (128)$$

is a four-dimensional orthonormal single-particle space.

Exact closure under the bath Hamiltonian. By construction,

$$h|c_s\rangle = sm|c_s\rangle + v|d_s\rangle. \quad (129)$$

Acting on the outer orbital gives

$$h|d_s\rangle = \frac{(h^2 - smh)|c_s\rangle}{v} \quad (130)$$

$$= \frac{\varepsilon^2|c_s\rangle - sm(sm|c_s\rangle + v|d_s\rangle)}{v} \quad (131)$$

$$= \frac{\varepsilon^2 - m^2}{v}|c_s\rangle - sm|d_s\rangle \quad (132)$$

$$= v|c_s\rangle - sm|d_s\rangle. \quad (133)$$

Hence each pair is invariant:

$$\boxed{h_s = h|_{\{c_s, d_s\}} = \begin{pmatrix} sm & v \\ v & -sm \end{pmatrix}.} \quad (134)$$

In particular,

$$h_s^2 = \varepsilon^2 I, \quad \text{spec}(h_s) = \{-\varepsilon, +\varepsilon\}. \quad (135)$$

The reduction retains both original band energies.

Define

$$\mathcal{P} = \sum_{s=\pm} (|c_s\rangle\langle c_s| + |d_s\rangle\langle d_s|). \quad (136)$$

Closure implies

$$(1 - \mathcal{P})h\mathcal{P} = 0. \quad (137)$$

Since $h = h^\dagger$,

$$\mathcal{P}h(1 - \mathcal{P}) = [(1 - \mathcal{P})h\mathcal{P}]^\dagger = 0. \quad (138)$$

Therefore,

$$\boxed{[h, \mathcal{P}] = 0, \quad h = \mathcal{P}h\mathcal{P} + (1 - \mathcal{P})h(1 - \mathcal{P}).} \quad (139)$$

The orthogonal complement is exactly decoupled.

Explicit support on the original lattice. For every rung, introduce

$$|j, s\rangle = \frac{|jA\rangle + is|jB\rangle}{\sqrt{2}}, \quad U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}. \quad (140)$$

The transformed matrices are

$$U^\dagger \tau_y U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad U^\dagger T U = \begin{pmatrix} 0 & 0 \\ -iv & 0 \end{pmatrix}. \quad (141)$$

Consequently,

$$h|j, +\rangle = m|j, +\rangle - iv|j - 1, -\rangle, \quad (142)$$

$$h|j, -\rangle = -m|j, -\rangle + iv|j + 1, +\rangle. \quad (143)$$

At the impurity rung,

$$\boxed{|c_\pm\rangle = |0, \pm\rangle, \quad |d_+\rangle = -i| -1, -\rangle, \quad |d_-\rangle = i|1, +\rangle.} \quad (144)$$

Thus the four active orbitals have support only on the central rung and its two neighboring rungs. In this local orbital basis, the bath consists of disconnected dimers. The impurity couples the two dimers that contain the central orbitals.

subsectionTransformation of the impurity exchange

The impurity spin couples equally to the two physical sites of rung $j = 0$:

$$H_K = J\mathbf{S}_d \cdot (\mathbf{s}_{0A} + \mathbf{s}_{0B}), \quad (145)$$

where

$$\mathbf{s}_{0A} = \frac{1}{2} \sum_{\sigma, \sigma'} a_{0\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} a_{0\sigma'}, \quad (146)$$

$$\mathbf{s}_{0B} = \frac{1}{2} \sum_{\sigma, \sigma'} b_{0\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} b_{0\sigma'}. \quad (147)$$

Here $\boldsymbol{\sigma}$ denotes the Pauli matrices acting on physical spin. The labels A, B and $+, -$ below refer to spatial orbitals, not to physical spin.

From orbital states to fermionic operators. The two central orbitals are

$$|c_s\rangle = \frac{|0A\rangle + is|0B\rangle}{\sqrt{2}}, \quad s = \pm 1. \quad (148)$$

For each physical spin σ , the associated creation operator is therefore

$$c_{s\sigma}^\dagger = \frac{a_{0\sigma}^\dagger + is b_{0\sigma}^\dagger}{\sqrt{2}}. \quad (149)$$

Taking the Hermitian conjugate gives

$$c_{s\sigma} = \frac{a_{0\sigma} - is b_{0\sigma}}{\sqrt{2}}. \quad (150)$$

In particular,

$$c_{+\sigma} = \frac{a_{0\sigma} - ib_{0\sigma}}{\sqrt{2}}, \quad c_{-\sigma} = \frac{a_{0\sigma} + ib_{0\sigma}}{\sqrt{2}}. \quad (151)$$

Adding and subtracting these equations yields the inverse transformation,

$$a_{0\sigma} = \frac{c_{+\sigma} + c_{-\sigma}}{\sqrt{2}}, \quad b_{0\sigma} = \frac{i(c_{+\sigma} - c_{-\sigma})}{\sqrt{2}}, \quad (152)$$

$$a_{0\sigma}^\dagger = \frac{c_{+\sigma}^\dagger + c_{-\sigma}^\dagger}{\sqrt{2}}, \quad b_{0\sigma}^\dagger = \frac{-i(c_{+\sigma}^\dagger - c_{-\sigma}^\dagger)}{\sqrt{2}}. \quad (153)$$

Equivalently, introducing orbital spinors

$$\Psi_{0\sigma} = \begin{pmatrix} a_{0\sigma} \\ b_{0\sigma} \end{pmatrix}, \quad C_\sigma = \begin{pmatrix} c_{+\sigma} \\ c_{-\sigma} \end{pmatrix}, \quad (154)$$

we have

$$\Psi_{0\sigma} = UC_\sigma, \quad U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \quad U^\dagger U = I_2. \quad (155)$$

Thus the transformation preserves the canonical anticommutation relations:

$$\{c_{s\sigma}, c_{s'\sigma'}^\dagger\} = \delta_{ss'}\delta_{\sigma\sigma'}, \quad \{c_{s\sigma}, c_{s'\sigma'}\} = 0. \quad (156)$$

Explicit transformation of the two local spins. Substituting Eqs. (152) and (153) into the spin on site A gives

$$\begin{aligned} \mathbf{s}_{0A} &= \frac{1}{4} \sum_{\sigma, \sigma'} \left(c_{+\sigma}^\dagger + c_{-\sigma}^\dagger \right) \boldsymbol{\sigma}_{\sigma\sigma'} (c_{+\sigma'} + c_{-\sigma'}) \\ &= \frac{1}{4} \sum_{\sigma, \sigma'} \left[c_{+\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{+\sigma'} + c_{-\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{-\sigma'} \right. \\ &\quad \left. + c_{+\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{-\sigma'} + c_{-\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{+\sigma'} \right]. \end{aligned} \quad (157)$$

For site B , the phase factors satisfy $(-i)i = 1$, so

$$\begin{aligned} \mathbf{s}_{0B} &= \frac{1}{4} \sum_{\sigma, \sigma'} \left(c_{+\sigma}^\dagger - c_{-\sigma}^\dagger \right) \boldsymbol{\sigma}_{\sigma\sigma'} (c_{+\sigma'} - c_{-\sigma'}) \\ &= \frac{1}{4} \sum_{\sigma, \sigma'} \left[c_{+\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{+\sigma'} + c_{-\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{-\sigma'} \right. \\ &\quad \left. - c_{+\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{-\sigma'} - c_{-\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{+\sigma'} \right]. \end{aligned} \quad (158)$$

The terms transferring an electron between the two central orbitals cancel when the two physical spins are added:

$$\mathbf{s}_{0A} + \mathbf{s}_{0B} = \frac{1}{2} \sum_{\sigma, \sigma'} \left[c_{+\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{+\sigma'} + c_{-\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{-\sigma'} \right]. \quad (159)$$

Defining

$$\mathbf{s}_{c_s} = \frac{1}{2} \sum_{\sigma, \sigma'} c_{s\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{s\sigma'}, \quad (160)$$

we obtain the exact operator identity

$$\boxed{\mathbf{s}_{0A} + \mathbf{s}_{0B} = \mathbf{s}_{c_+} + \mathbf{s}_{c_-}}. \quad (161)$$

No reordering of fermionic operators is required in this calculation: each bilinear retains a creation operator followed by an annihilation operator.

Consequently, the impurity exchange becomes

$$\boxed{H_K = J \mathbf{S}_d \cdot (\mathbf{s}_{c_+} + \mathbf{s}_{c_-})}. \quad (162)$$

In particular, the exchange coefficient remains J ; the factors from the orbital transformation do not produce an additional factor of $1/2$ in Eq. (162).

Spin-conserving and spin-flip terms. For each central orbital,

$$s_{c_s}^z = \frac{1}{2} (n_{c_s\uparrow} - n_{c_s\downarrow}), \quad (163)$$

$$s_{c_s}^+ = c_{s\uparrow}^\dagger c_{s\downarrow}, \quad s_{c_s}^- = c_{s\downarrow}^\dagger c_{s\uparrow}. \quad (164)$$

Using

$$\mathbf{S}_d \cdot \mathbf{s}_{c_s} = S_d^z s_{c_s}^z + \frac{1}{2} (S_d^+ s_{c_s}^- + S_d^- s_{c_s}^+), \quad (165)$$

the exchange can be written explicitly as

$$\boxed{H_K = \frac{J}{2} \sum_{s=\pm} \left[S_d^z (n_{c_s\uparrow} - n_{c_s\downarrow}) \right. \\ \left. + S_d^+ c_{s\downarrow}^\dagger c_{s\uparrow} + S_d^- c_{s\uparrow}^\dagger c_{s\downarrow} \right]}. \quad (166)$$

The spin-flip terms exchange angular momentum between the impurity and an electron within the same central orbital. They do not transfer electrons between c_+ and c_- .

Why equal exchange couplings are essential. The cancellation can be checked by temporarily allowing different couplings:

$$H_K = \mathbf{S}_d \cdot (J_A \mathbf{s}_{0A} + J_B \mathbf{s}_{0B}). \quad (167)$$

Equations (157) and (158) then give

$$H_K = \frac{J_A + J_B}{2} \mathbf{S}_d \cdot (\mathbf{s}_{c+} + \mathbf{s}_{c-}) + \frac{J_A - J_B}{4} \mathbf{S}_d \cdot \sum_{\sigma, \sigma'} \left[c_{+\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{-\sigma'} + c_{-\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{+\sigma'} \right]. \quad (168)$$

Thus the orbital-transfer exchange terms vanish precisely for $J_A = J_B$. In the following, we retain this symmetric choice, $J_A = J_B = J$.

The fermionic operators associated with the outer orbitals are defined by

$$d_{s\sigma}^\dagger |\text{vac}\rangle = |d_s\rangle \otimes |\sigma\rangle, \quad d_{s\sigma} = (d_{s\sigma}^\dagger)^\dagger, \quad (169)$$

where $s = \pm 1$ labels the orbital and $\sigma = \uparrow, \downarrow$ denotes physical spin.

To write these operators explicitly, introduce the rotated orbitals on an arbitrary rung:

$$f_{js\sigma}^\dagger = \frac{a_{j\sigma}^\dagger + is b_{j\sigma}^\dagger}{\sqrt{2}}, \quad f_{js\sigma} = \frac{a_{j\sigma} - is b_{j\sigma}}{\sqrt{2}}. \quad (170)$$

The central operators satisfy $c_{s\sigma}^\dagger = f_{0s\sigma}^\dagger$. Using

$$|d_+\rangle = -i| -1, -\rangle, \quad |d_-\rangle = i|1, +\rangle, \quad (171)$$

the outer creation operators are

$$d_{+\sigma}^\dagger = -i f_{-1, -, \sigma}^\dagger = \frac{-ia_{-1, \sigma}^\dagger - b_{-1, \sigma}^\dagger}{\sqrt{2}}, \quad (172)$$

$$d_{-\sigma}^\dagger = i f_{1, +, \sigma}^\dagger = \frac{ia_{1, \sigma}^\dagger - b_{1, \sigma}^\dagger}{\sqrt{2}}. \quad (173)$$

Taking Hermitian conjugates gives

$$d_{+\sigma} = i f_{-1, -, \sigma} = \frac{ia_{-1, \sigma} - b_{-1, \sigma}}{\sqrt{2}}, \quad (174)$$

$$d_{-\sigma} = -i f_{1, +, \sigma} = \frac{-ia_{1, \sigma} - b_{1, \sigma}}{\sqrt{2}}. \quad (175)$$

Thus each d operator describes a definite orbital combination on a neighboring rung, rather than an additional physical lattice site.

The orthonormality of the active spatial orbitals implies

$$\{d_{s\sigma}, d_{s'\sigma'}^\dagger\} = \delta_{ss'} \delta_{\sigma\sigma'}, \quad \{c_{s\sigma}, d_{s'\sigma'}^\dagger\} = 0. \quad (176)$$

We denote their occupation operators by

$$n_{d_s\sigma} = d_{s\sigma}^\dagger d_{s\sigma}, \quad n_{d_s} = \sum_{\sigma} n_{d_s\sigma}. \quad (177)$$

With these phase conventions, the hopping between the central and outer orbitals is real:

$$H_{\text{hop,act}} = v \sum_{s=\pm 1} \sum_{\sigma} (c_{s\sigma}^\dagger d_{s\sigma} + d_{s\sigma}^\dagger c_{s\sigma}), \quad v = 2t. \quad (178)$$

Restriction to the active orbitals is exact. The inverse transformation expresses both physical impurity-coupled operators $a_{0\sigma}$ and $b_{0\sigma}$ entirely in terms of $c_{+\sigma}$ and $c_{-\sigma}$. Therefore, H_K contains no operators belonging to the orthogonal complement of the active subspace.

The outer orbitals $d_{\pm}$ do not appear directly in H_K . They participate through the bath hopping,

$$H_{0,\text{act}} = \sum_{s=\pm 1} \sum_{\sigma} \left[sm (c_{s\sigma}^{\dagger} c_{s\sigma} - d_{s\sigma}^{\dagger} d_{s\sigma}) + v (c_{s\sigma}^{\dagger} d_{s\sigma} + d_{s\sigma}^{\dagger} c_{s\sigma}) \right], \quad v = 2t. \quad (179)$$

Combining the bath and exchange terms yields

$$\boxed{H_{\text{act}} = H_{0,\text{act}} + J \mathbf{S}_d \cdot (\mathbf{s}_{c_+} + \mathbf{s}_{c_-})}. \quad (180)$$

Since the active single-particle subspace is invariant under h , the full Hamiltonian decomposes as

$$H = H_{\text{act}} + H_{\text{dark}}, \quad (181)$$

where H_{dark} contains only decoupled bath orbitals. This is an exact change of orbital basis: no expansion in J , elimination of virtual excitations, or projection onto a single energy band has been used.

The decoupled bath Hamiltonian To obtain H_{dark} explicitly, we perform the same orbital rotation on every rung:

$$f_{js\sigma}^{\dagger} = \frac{a_{j\sigma}^{\dagger} + is b_{j\sigma}^{\dagger}}{\sqrt{2}}, \quad s = \pm 1. \quad (182)$$

For the annihilation operators, this gives

$$\Psi_{j\sigma} = U F_{j\sigma}, \quad F_{j\sigma} = \begin{pmatrix} f_{j,+, \sigma} \\ f_{j, -, \sigma} \end{pmatrix}, \quad U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}. \quad (183)$$

Transformation of the full bath. The original bath Hamiltonian is

$$H_0 = \sum_{j,\sigma} \left[\Psi_{j\sigma}^{\dagger} T \Psi_{j+1,\sigma} + \text{H.c.} + \Psi_{j\sigma}^{\dagger} m \tau_y \Psi_{j\sigma} \right], \quad T = t(-\tau_x - i\tau_z). \quad (184)$$

The transformed matrices are

$$U^{\dagger} (m \tau_y) U = \begin{pmatrix} m & 0 \\ 0 & -m \end{pmatrix}, \quad U^{\dagger} T U = \begin{pmatrix} 0 & 0 \\ -iv & 0 \end{pmatrix}, \quad v = 2t. \quad (185)$$

Consequently,

$$H_0 = \sum_{j,\sigma} \left[m (n_{j,+, \sigma} - n_{j, -, \sigma}) - iv f_{j, -, \sigma}^{\dagger} f_{j+1, +, \sigma} + iv f_{j+1, +, \sigma}^{\dagger} f_{j, -, \sigma} \right], \quad (186)$$

where

$$n_{j,s,\sigma} = f_{j,s,\sigma}^{\dagger} f_{j,s,\sigma}. \quad (187)$$

For periodic boundary conditions,

$$\sum_j n_{j,+,\sigma} = \sum_j n_{j+1,+,\sigma}. \quad (188)$$

We may therefore regroup Eq. (186) into independent dimers:

$$\boxed{H_0 = \sum_j H_j^{\text{dim}},} \quad (189)$$

with

$$H_j^{\text{dim}} = \sum_{\sigma} \left[m(n_{j+1,+,\sigma} - n_{j,-,\sigma}) - iv f_{j,-,\sigma}^{\dagger} f_{j+1,+,\sigma} + iv f_{j+1,+,\sigma}^{\dagger} f_{j,-,\sigma} \right]. \quad (190)$$

Each term acts only on the two spatial orbitals

$$\mathcal{D}_j = \text{span}\{|j, -\rangle, |j+1, +\rangle\}. \quad (191)$$

Every rotated orbital belongs to exactly one such dimer: $|j, -\rangle$ belongs to $\mathcal{D}_j$, whereas $|j, +\rangle$ belongs to $\mathcal{D}_{j-1}$. Hence no orbital is counted twice.

Identification of the impurity-active dimers. The central orbitals are

$$c_{+\sigma} = f_{0,+,\sigma}, \quad c_{-\sigma} = f_{0,-,\sigma}. \quad (192)$$

They belong to $\mathcal{D}_{-1}$ and $\mathcal{D}_0$, respectively. Thus

$$\mathcal{K}_0 = \mathcal{D}_{-1} \oplus \mathcal{D}_0, \quad H_{0,\text{act}} = H_{-1}^{\text{dim}} + H_0^{\text{dim}}. \quad (193)$$

Using

$$d_{+\sigma} = i f_{-1,-,\sigma}, \quad d_{-\sigma} = -i f_{1,+,\sigma}, \quad (194)$$

these two terms become

$$H_{-1}^{\text{dim}} = \sum_{\sigma} \left[m(n_{c_{+\sigma}} - n_{d_{+\sigma}}) + v(c_{+\sigma}^{\dagger} d_{+\sigma} + d_{+\sigma}^{\dagger} c_{+\sigma}) \right], \quad (195)$$

$$H_0^{\text{dim}} = \sum_{\sigma} \left[-m(n_{c_{-\sigma}} - n_{d_{-\sigma}}) + v(c_{-\sigma}^{\dagger} d_{-\sigma} + d_{-\sigma}^{\dagger} c_{-\sigma}) \right]. \quad (196)$$

The remaining dimers constitute the dark bath:

$$\boxed{H_{\text{dark}} = \sum_{j \neq -1, 0} H_j^{\text{dim}}.} \quad (197)$$

Explicitly,

$$\boxed{H_{\text{dark}} = \sum_{\substack{j \neq -1, 0 \\ \sigma}} \left[m \left(f_{j+1,+,\sigma}^{\dagger} f_{j+1,+,\sigma} - f_{j,-,\sigma}^{\dagger} f_{j,-,\sigma} \right) - iv f_{j,-,\sigma}^{\dagger} f_{j+1,+,\sigma} + iv f_{j+1,+,\sigma}^{\dagger} f_{j,-,\sigma} \right].} \quad (198)$$

Although neighboring dimers can share a physical rung, they contain different orthogonal orbital combinations. The dark orbitals therefore do not overlap with the four active orbitals. Since the impurity exchange contains only $c_{+\sigma}$ and $c_{-\sigma}$,

$$H_{\text{act}} = H_{-1}^{\text{dim}} + H_0^{\text{dim}} + J\mathbf{S}_d \cdot (\mathbf{s}_{c_+} + \mathbf{s}_{c_-}), \quad (199)$$

and the full Hamiltonian satisfies

$$\boxed{H = H_{\text{act}} + H_{\text{dark}}, \quad [H_{\text{act}}, H_{\text{dark}}] = 0.} \quad (200)$$

Diagonal form of the dark bath. For each dark dimer, introduce

$$p_{j\sigma} = f_{j+1,+, \sigma}, \quad q_{j\sigma} = if_{j,-, \sigma}. \quad (201)$$

Then

$$H_j^{\text{dim}} = \sum_{\sigma} \begin{pmatrix} p_{j\sigma}^{\dagger} & q_{j\sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} m & v \\ v & -m \end{pmatrix} \begin{pmatrix} p_{j\sigma} \\ q_{j\sigma} \end{pmatrix}. \quad (202)$$

Writing

$$\varepsilon = \sqrt{m^2 + v^2}, \quad u = \sqrt{\frac{\varepsilon + m}{2\varepsilon}}, \quad w = \sqrt{\frac{\varepsilon - m}{2\varepsilon}}, \quad (203)$$

the eigenmode operators are

$$\gamma_{j,+, \sigma} = up_{j\sigma} + wq_{j\sigma}, \quad (204)$$

$$\gamma_{j,-, \sigma} = -wp_{j\sigma} + uq_{j\sigma}. \quad (205)$$

They diagonalize the dimer Hamiltonian:

$$H_j^{\text{dim}} = \varepsilon \sum_{\sigma} \left(\gamma_{j,+, \sigma}^{\dagger} \gamma_{j,+, \sigma} - \gamma_{j,-, \sigma}^{\dagger} \gamma_{j,-, \sigma} \right). \quad (206)$$

Therefore,

$$\boxed{H_{\text{dark}} = \varepsilon \sum_{\substack{j \neq -1, 0 \\ \sigma}} (n_{j,+, \sigma}^{\gamma} - n_{j,-, \sigma}^{\gamma})}. \quad (207)$$

The dark bath consists of $L - 2$ independent dimers, each with spin-degenerate single-particle energies $-\varepsilon$ and $+\varepsilon$.

Energy contribution for a filled lower dark band. If every lower dark eigenmode is occupied by both spins and every upper dark eigenmode is empty, then

$$|\text{FB}\rangle_{\text{dark}} = \prod_{j \neq -1, 0} \gamma_{j,-, \uparrow}^{\dagger} \gamma_{j,-, \downarrow}^{\dagger} |\text{vac}\rangle_{\text{dark}}, \quad (208)$$

with

$$N_{\text{dark}} = 2(L - 2), \quad \boxed{E_{\text{dark}} = -2\varepsilon(L - 2)}. \quad (209)$$

At total filling $N_e = 2L$, this occupation leaves four electrons in the active orbitals. Within this sector,

$$E_{\text{tot}} = E_{\text{act}}(N_{\text{act}} = 4) - 2\varepsilon(L - 2). \quad (210)$$

This constant energy shift follows from the specified dark-band occupation; it is not the operator H_{dark} itself.

If the global ground state is sought without fixing the active particle number, the allowed particle allocations must instead be compared:

$$E_0(N_e) = \min_{N_{\text{act}}} [E_{\text{act}}(N_{\text{act}}) + E_{\text{dark}}(N_e - N_{\text{act}})]. \quad (211)$$

D.2 Competing local ground states and their energy criterion

We retain the definitions

$$m = \alpha t, \quad v = 2t, \quad \varepsilon = \sqrt{m^2 + v^2}, \quad (212)$$

and take $m \geq 0$ and $J > 0$. The active Hamiltonian is

$$H_{\text{act}} = H_J + H_m + V, \quad (213)$$

where

$$H_J = J \mathbf{S}_d \cdot (\mathbf{s}_{c_+} + \mathbf{s}_{c_-}), \quad (214)$$

$$H_m = m(n_{c_+} - n_{c_-} - n_{d_+} + n_{d_-}), \quad (215)$$

$$V = \sum_{s=\pm} V_s, \quad (216)$$

$$V_s = v \sum_{\sigma} (c_{s\sigma}^\dagger d_{s\sigma} + d_{s\sigma}^\dagger c_{s\sigma}). \quad (217)$$

The two dimer charges are separately conserved:

$$N_s = n_{c_s} + n_{d_s}, \quad [H_{\text{act}}, N_s] = 0. \quad (218)$$

Dark-bath contribution and particle allocation. For a filled lower dark band,

$$N_{\text{dark}}^{(0)} = 2(L - 2), \quad E_{\text{dark}}^{(0)} = -2(L - 2)\varepsilon. \quad (219)$$

At total particle number $N_e = 2L$, this leaves $N_{\text{act}} = 4$ electrons in the active orbitals.

More generally, changing the active particle number requires removing electrons from the dark lower band or adding them to the dark upper band. For the system sizes considered here,

$$E_{\text{dark}}(N_{\text{act}}) = E_{\text{dark}}^{(0)} + \varepsilon |N_{\text{act}} - 4|. \quad (220)$$

Let $E_{n_+, n_-}^{\text{act}}$ denote the lowest eigenvalue of the full active Hamiltonian in the charge sector $(N_+, N_-) = (n_+, n_-)$. The exact ground-state energy is

$$E_{\text{GS}} = E_{\text{dark}}^{(0)} + \min_{0 \leq n_+, n_- \leq 4} \left[E_{n_+, n_-}^{\text{act}} + \varepsilon |n_+ + n_- - 4| \right]. \quad (221)$$

Central strong-exchange doublet. We first analyze the controlled regime

$$v, m \ll J/4. \quad (222)$$

With one electron on each central orbital, define

$$\mathbf{T} = \mathbf{s}_{c_+} + \mathbf{s}_{c_-}, \quad \mathbf{F} = \mathbf{S}_d + \mathbf{T}. \quad (223)$$

The exchange energy follows from angular-momentum addition:

$$H_J = \frac{J}{2} (\mathbf{F}^2 - \mathbf{T}^2 - \mathbf{S}_d^2), \quad (224)$$

$$E_J(T, F) = \frac{J}{2} \left[F(F + 1) - T(T + 1) - \frac{3}{4} \right]. \quad (225)$$

The possible multiplets have energies

$$\begin{array}{c|c|c} T & F & E_J \\ \hline 1 & 1/2 & -J \\ 1 & 3/2 & J/2 \\ 0 & 1/2 & 0 \end{array} . \quad (226)$$

The lowest central multiplet is therefore a doublet formed by the central-electron triplet and the impurity spin.

Explicitly, define

$$|T_+\rangle = |\uparrow_+\uparrow_-\rangle_c, \quad (227)$$

$$|T_0\rangle = \frac{|\uparrow_+\downarrow_-\rangle_c + |\downarrow_+\uparrow_-\rangle_c}{\sqrt{2}}, \quad (228)$$

$$|T_-\rangle = |\downarrow_+\downarrow_-\rangle_c. \quad (229)$$

A consistent choice of doublet states is

$$|F_+\rangle = \sqrt{\frac{2}{3}}|\downarrow\rangle_{\text{imp}}|T_+\rangle - \sqrt{\frac{1}{3}}|\uparrow\rangle_{\text{imp}}|T_0\rangle, \quad (230)$$

$$|F_-\rangle = \sqrt{\frac{1}{3}}|\downarrow\rangle_{\text{imp}}|T_0\rangle - \sqrt{\frac{2}{3}}|\uparrow\rangle_{\text{imp}}|T_-\rangle. \quad (231)$$

Let P project onto this central doublet, with the outer orbitals unrestricted. Then

$$PH_J P = -JP, \quad Pn_{c_+}P = Pn_{c_-}P = P. \quad (232)$$

Consequently,

$$PH_m P = -m(n_{d_+} - n_{d_-})P. \quad (233)$$

A single hopping event changes a central occupation from one to zero or two, and hence leaves the retained doublet:

$$PVP = 0. \quad (234)$$

D.3 Second-order coupling to an outer spin

We treat the hopping between the central and outer orbitals as a perturbation to the strong central exchange. Consider first the outer orbital d_+ :

$$V_+ = v \sum_{\sigma} \left(c_{+\sigma}^\dagger d_{+\sigma} + d_{+\sigma}^\dagger c_{+\sigma} \right). \quad (235)$$

The unperturbed central ground states are the doublet $|F_\pm\rangle$, with energy $E_0 = -J$ and occupations $n_{c_+} = n_{c_-} = 1$.

A single hop changes n_{c_+} from one to zero or two. It therefore takes the state outside the central ground-state doublet. All matrix elements of V_+ within the retained low-energy space vanish, so the first-order correction is zero.

The leading correction comes from a virtual hop out of the low-energy space followed by a hop back. For a low-energy state $|\psi\rangle$, second-order perturbation theory gives

$$\boxed{\delta E_\psi^{(2)} = - \sum_n \frac{|\langle n|V_+|\psi\rangle|^2}{E_n - E_0}}. \quad (236)$$

We evaluate this expression separately in the singlet and triplet sectors of the central doublet and the outer spin. Spin-rotation symmetry prevents these sectors from mixing.

Energies of the intermediate states. First find $E_n - E_0$, to find nonzero numerator, n should belong to sector $(0, 1), (2, 1), (1, 0), (1, 2)$ of H_J

After one hop, c_+ is either empty or doubly occupied, and hence carries no spin. The impurity then couples only to the electron on c_- :

$$H_J^{\text{int}} = J\mathbf{S}_d \cdot \mathbf{s}_{c_-}. \quad (237)$$

These two spins form either a singlet or a triplet:

$$E_{\text{int},0} = -\frac{3J}{4}, \quad E_{\text{int},1} = \frac{J}{4}. \quad (238)$$

Relative to $E_0 = -J$, the excitation energies are

$$\boxed{\delta_0 = \frac{J}{4}, \quad \delta_1 = \frac{5J}{4}.} \quad (239)$$

Here we neglect the orbital-energy corrections to these denominators, which is justified for $m, v \ll J/4$.

Which spin configurations can hop? Suppose that d_+ is singly occupied. The hopping pair (c_+, d_+) initially contains two electrons. A doubly occupied spatial orbital is a spin singlet. Since hopping conserves spin, only the singlet component of this pair can hop into an empty–doubly occupied configuration.

Define

$$|s_{c_+, d_+}\rangle = \frac{|\uparrow\rangle_{c_+} |\downarrow\rangle_{d_+} - |\downarrow\rangle_{c_+} |\uparrow\rangle_{d_+}}{\sqrt{2}}. \quad (240)$$

The two possible final charge configurations are $|D_{c_+}, 0_{d_+}\rangle$ and $|0_{c_+}, D_{d_+}\rangle$. Each has a hopping amplitude of magnitude $\sqrt{2}v$, so their total squared amplitude is

$$\boxed{\|V_+ |s_{c_+, d_+}\rangle\|^2 = 4v^2.} \quad (241)$$

Energy correction in the singlet sector. The central doublet and the outer spin form the singlet

$$|\Sigma\rangle = \frac{|F_+\rangle |\downarrow\rangle_{d_+} - |F_-\rangle |\uparrow\rangle_{d_+}}{\sqrt{2}}. \quad (242)$$

To determine its hopping amplitude, we extract its (c_+, d_+) singlet component. Substituting the explicit expressions for $|F_{\pm}\rangle$ gives

$${}_{c_+, d_+} \langle s | \Sigma \rangle = -\frac{\sqrt{3}}{2} |s_{\text{imp}, c_-}\rangle, \quad (243)$$

where

$$|s_{\text{imp}, c_-}\rangle = \frac{|\uparrow\rangle_{\text{imp}} |\downarrow\rangle_{c_-} - |\downarrow\rangle_{\text{imp}} |\uparrow\rangle_{c_-}}{\sqrt{2}}. \quad (244)$$

Thus the hopping-pair singlet has probability $3/4$, and the remaining impurity–electron pair is also a singlet. Combining this probability with Eq. (241),

$$\sum_{n \in \text{singlet}} |\langle n | V_+ | \Sigma \rangle|^2 = \frac{3}{4} (4v^2) = 3v^2. \quad (245)$$

Using the denominator $\delta_0 = J/4$,

$$\boxed{\delta E_{\Sigma}^{(2)} = -\frac{3v^2}{J/4} = -12 \frac{v^2}{J}.} \quad (246)$$

Energy correction in the triplet sector. Choose the highest component of the triplet:

$$|\mathcal{T}_1\rangle = |F_+\rangle |\uparrow\rangle_{d_+}. \quad (247)$$

Because the outer spin is up, only the component with a down spin on c_+ contributes to the hopping-pair singlet. In $|F_+\rangle$, this component is

$$-\frac{1}{\sqrt{6}} |\uparrow\rangle_{\text{imp}} |\downarrow\rangle_{c_+} |\uparrow\rangle_{c_-}. \quad (248)$$

Its overlap with the pair singlet is therefore

$$\begin{aligned} {}_{c_+, d_+} \langle s | \mathcal{T}_1 \rangle &= \left(-\frac{1}{\sqrt{6}} \right) \left(-\frac{1}{\sqrt{2}} \right) |\uparrow\rangle_{\text{imp}} |\uparrow\rangle_{c_-} \\ &= \frac{1}{\sqrt{12}} |\uparrow\rangle_{\text{imp}} |\uparrow\rangle_{c_-}. \end{aligned} \quad (249)$$

The hopping-pair singlet probability is $1/12$, and the remaining impurity–electron pair is a triplet. Consequently,

$$\sum_{n \in \text{triplet}} |\langle n | V_+ | \mathcal{T}_1 \rangle|^2 = \frac{1}{12} (4v^2) = \frac{v^2}{3}. \quad (250)$$

Using $\delta_1 = 5J/4$ gives

$$\boxed{\delta E_{\mathcal{T}}^{(2)} = -\frac{v^2/3}{5J/4} = -\frac{4}{15} \frac{v^2}{J}}. \quad (251)$$

D.4 Second-order energy matrix and the local level crossing

We work in the strong-exchange regime

$$v, m \ll J/4, \quad v = 2t, \quad m = \alpha t. \quad (252)$$

The retained central states are the doublet $|F_{\pm}\rangle$, with energy $E_0 = -J$ and occupations $n_{c_+} = n_{c_-} = 1$. In the four-electron active sector, the remaining two electrons occupy the outer orbitals d_+ and d_- .

Low-energy basis. In the sector

$$S_{\text{tot}}^z = F^z + s_{d_+}^z + s_{d_-}^z = \frac{1}{2}, \quad (253)$$

choose the orthonormal basis

$$|1\rangle = |F_-\rangle |\uparrow_+ \uparrow_-\rangle_{\text{out}}, \quad (254)$$

$$|2\rangle = |F_+\rangle |\downarrow_+ \uparrow_-\rangle_{\text{out}}, \quad (255)$$

$$|3\rangle = |F_+\rangle |\uparrow_+ \downarrow_-\rangle_{\text{out}}, \quad (256)$$

$$|4\rangle = |F_+\rangle |D_+, 0_-\rangle, \quad (257)$$

$$|5\rangle = |F_+\rangle |0_+, D_-\rangle, \quad (258)$$

where

$$|D_+, 0_-\rangle = d_{+\uparrow}^\dagger d_{+\downarrow}^\dagger |0\rangle_{\text{out}}, \quad |0_+, D_-\rangle = d_{-\uparrow}^\dagger d_{-\downarrow}^\dagger |0\rangle_{\text{out}}. \quad (259)$$

The first three states belong to the charge sector $(N_+, N_-) = (2, 2)$, while $|4\rangle$ and $|5\rangle$ belong to $(3, 1)$ and $(1, 3)$, respectively.

Second-order perturbation matrix. The full hopping perturbation is

$$V = V_+ + V_-, \quad V_s = v \sum_{\sigma} (c_{s\sigma}^\dagger d_{s\sigma} + d_{s\sigma}^\dagger c_{s\sigma}). \quad (260)$$

Since one hop changes a central occupation from one to zero or two, its matrix elements within the retained space vanish. The leading hopping correction is therefore the second-order matrix

$$W_{ij} = - \sum_{n \notin \mathcal{P}} \frac{\langle i | V | n \rangle \langle n | V | j \rangle}{E_n^{(0)} - E_0}. \quad (261)$$

Here $\mathcal{P}$ denotes the retained many-body subspace, and $|n\rangle$ are eigenstates of H_J outside that subspace. At this order, the orbital-energy corrections to the denominators are neglected.

Expanding $V = V_+ + V_-$ gives

$$W = W_{++} + W_{--} + W_{+-} + W_{-+}. \quad (262)$$

The mixed terms vanish. After a hop in one channel, a hop in the other channel cannot restore both central occupations to one. Moreover, H_J conserves each central occupation, so the intermediate-state resolvent cannot restore them either. Hence

$$W_{+-} = W_{-+} = 0, \quad \boxed{W = W_{++} + W_{--}}. \quad (263)$$

Matrix elements from the single-side calculation. For a singly occupied outer orbital, the previously calculated singlet and triplet energy shifts are

$$e_S = -12 \frac{v^2}{J}, \quad e_T = -\frac{4}{15} \frac{v^2}{J}. \quad (264)$$

The empty and doubly occupied outer orbitals have the common shift

$$C_* = -\frac{(3/4)v^2}{J/4} - \frac{(1/4)v^2}{5J/4} = -\frac{16}{5} \frac{v^2}{J}. \quad (265)$$

To express the singly occupied result in a product-spin basis, use

$$|S\rangle = \frac{|F_+\rangle |\downarrow\rangle - |F_-\rangle |\uparrow\rangle}{\sqrt{2}}, \quad (266)$$

$$|T_0\rangle = \frac{|F_+\rangle |\downarrow\rangle + |F_-\rangle |\uparrow\rangle}{\sqrt{2}}. \quad (267)$$

Thus the matrix on the two antiparallel product states is

$$\begin{pmatrix} A & B \\ B & A \end{pmatrix}, \quad A = \frac{e_S + e_T}{2}, \quad B = \frac{e_T - e_S}{2}. \quad (268)$$

A parallel product state is a triplet and has shift e_T .

For two hops on the $+$ side, the $-$ outer state remains unchanged. In the five-state basis above,

$$W_{++} = \begin{pmatrix} A & B & 0 & 0 & 0 \\ B & A & 0 & 0 & 0 \\ 0 & 0 & e_T & 0 & 0 \\ 0 & 0 & 0 & C_* & 0 \\ 0 & 0 & 0 & 0 & C_* \end{pmatrix}. \quad (269)$$

Similarly, two hops on the $-$ side give

$$W_{--} = \begin{pmatrix} A & 0 & B & 0 & 0 \\ 0 & e_T & 0 & 0 & 0 \\ B & 0 & A & 0 & 0 \\ 0 & 0 & 0 & C_* & 0 \\ 0 & 0 & 0 & 0 & C_* \end{pmatrix}. \quad (270)$$

Adding the two matrices yields

$$W = \begin{pmatrix} 2A & B & B & 0 & 0 \\ B & A + e_T & 0 & 0 & 0 \\ B & 0 & A + e_T & 0 & 0 \\ 0 & 0 & 0 & 2C_* & 0 \\ 0 & 0 & 0 & 0 & 2C_* \end{pmatrix}. \quad (271)$$

Substituting the energy shifts gives the explicit result

$$W = \frac{v^2}{15J} \begin{pmatrix} -184 & 88 & 88 & 0 & 0 \\ 88 & -96 & 0 & 0 & 0 \\ 88 & 0 & -96 & 0 & 0 \\ 0 & 0 & 0 & -96 & 0 \\ 0 & 0 & 0 & 0 & -96 \end{pmatrix}. \quad (272)$$

The charge sectors do not mix because the original Hamiltonian conserves N_+ and N_- separately.

Including the orbital energies. Within the central doublet, $n_{c+} = n_{c-} = 1$, so

$$H_m \longrightarrow -m(n_{d+} - n_{d-}). \quad (273)$$

Its matrix in the chosen basis is

$$D = \text{diag}(0, 0, 0, -2m, +2m). \quad (274)$$

The active energy matrix through the retained order is therefore

$$\boxed{\mathcal{M} = -JI_5 + D + W.} \quad (275)$$

Its eigenvalues give the active energies up to corrections of order

$$O\left(\frac{v^2 m}{J^2}, \frac{v^4}{J^3}\right). \quad (276)$$

Diagonalization of the 22 block. The first three basis states form the 22 block:

$$\mathcal{M}_{22} = -JI_3 + \frac{v^2}{15J}\mathcal{A}, \quad \mathcal{A} = \begin{pmatrix} -184 & 88 & 88 \\ 88 & -96 & 0 \\ 88 & 0 & -96 \end{pmatrix}. \quad (277)$$

The antisymmetric vector

$$|a\rangle = \frac{|2\rangle - |3\rangle}{\sqrt{2}} \quad (278)$$

is an eigenvector of $\mathcal{A}$ with eigenvalue -96 .

The remaining subspace is spanned by

$$|1\rangle, \quad |s\rangle = \frac{|2\rangle + |3\rangle}{\sqrt{2}}. \quad (279)$$

In this basis,

$$\mathcal{A}_{\text{sym}} = \begin{pmatrix} -184 & 88\sqrt{2} \\ 88\sqrt{2} & -96 \end{pmatrix}. \quad (280)$$

Its characteristic equation is

$$0 = (-184 - \lambda)(-96 - \lambda) - 2(88)^2 \quad (281)$$

$$= \lambda^2 + 280\lambda + 2176 \quad (282)$$

$$= (\lambda + 272)(\lambda + 8). \quad (283)$$

Thus the three eigenvalues of $\mathcal{A}$ are

$$\boxed{\lambda = -272, -96, -8.} \quad (284)$$

The lowest active energy in the 22 sector is

$$\boxed{E_{22}^{\text{act}} = -J - \frac{272}{15} \frac{v^2}{J}.} \quad (285)$$

Its normalized eigenvector is

$$|\Psi_{22,+}^{(0)}\rangle = \sqrt{\frac{2}{3}}|1\rangle - \frac{1}{\sqrt{6}}|2\rangle - \frac{1}{\sqrt{6}}|3\rangle \quad (286)$$

$$\begin{aligned} &= \sqrt{\frac{2}{3}}|F_-\rangle|\uparrow_+\uparrow_-\rangle_{\text{out}} \\ &\quad - \frac{1}{\sqrt{6}}|F_+\rangle(|\downarrow_+\uparrow_-\rangle_{\text{out}} + |\uparrow_+\downarrow_-\rangle_{\text{out}}). \end{aligned} \quad (287)$$

The closed-shell sectors. The fourth and fifth basis states are already separate one-dimensional blocks of $\mathcal{M}$. Their energies are

$$\boxed{E_{31}^{\text{act}} = -J - \frac{96}{15} \frac{v^2}{J} - 2m,} \quad (288)$$

and

$$E_{13}^{\text{act}} = -J - \frac{96}{15} \frac{v^2}{J} + 2m. \quad (289)$$

Their leading-order states are

$$|\Psi_{31,+}^{(0)}\rangle = |F_+\rangle|D_+, 0_-\rangle, \quad |\Psi_{13,+}^{(0)}\rangle = |F_+\rangle|0_+, D_-\rangle. \quad (290)$$

For $m > 0$, the 13 branch lies above the 31 branch by $4m$ at this order.

Energy comparison. All three charge sectors considered here contain four active electrons. Their dark-bath contribution is therefore identical:

$$E_{\text{dark}}^{(0)} = -2(L-2)\varepsilon, \quad \varepsilon = \sqrt{m^2 + v^2}. \quad (291)$$

Adding this common contribution gives

$$E_{22} = -2(L-2)\varepsilon - J - \frac{272}{15} \frac{v^2}{J}, \quad (292)$$

$$E_{31} = -2(L-2)\varepsilon - J - \frac{96}{15} \frac{v^2}{J} - 2m. \quad (293)$$

Their difference is

$$E_{22} - E_{31} = 2m - \frac{176}{15} \frac{v^2}{J} + O\left(\frac{v^2 m}{J^2}, \frac{v^4}{J^3}\right). \quad (294)$$

Thus the leading-order criterion is

$$\begin{cases} \frac{176v^2}{15J} > 2m : & E_{22} < E_{31}, \\ \frac{176v^2}{15J} < 2m : & E_{31} < E_{22}. \end{cases} \quad (295)$$

The leading crossing position follows directly:

$$J_c^{(0)} = \frac{88}{15} \frac{v^2}{m} = \frac{352}{15\alpha} t. \quad (296)$$

This expression is controlled near $\alpha = 0^+$, where the crossing occurs in the strong-exchange regime. For general parameters, higher-order corrections and other active-particle-number sectors must also be checked before identifying the global ground-state boundary.

The entire calculation consists of constructing the second-order matrix, adding the projected orbital energies, and comparing its lowest eigenvalues. No additional interaction is introduced.

D.5 Structure and properties of the competing states

The labels (N_+, N_-) specify the conserved electron numbers of the two active dimers:

$$N_s = n_{c_s} + n_{d_s}. \quad (297)$$

In the strong-exchange low-energy space, the central orbitals are singly occupied and form the doublet $|F_{\pm}\rangle$ together with the impurity. The competing states differ in the occupation and spin configuration of the two outer electrons.

The balanced 22 state. For $n_{d_+} = n_{d_-} = 1$, the two outer spins form a triplet:

$$|R_+\rangle = |\uparrow_+\uparrow_-\rangle_{\text{out}}, \quad (298)$$

$$|R_0\rangle = \frac{|\uparrow_+\downarrow_-\rangle_{\text{out}} + |\downarrow_+\uparrow_-\rangle_{\text{out}}}{\sqrt{2}}, \quad (299)$$

$$|R_-\rangle = |\downarrow_+\downarrow_-\rangle_{\text{out}}. \quad (300)$$

Combining this triplet with the central spin $F = 1/2$ gives the lowest doublet

$$|\Psi_{22,+}^{(0)}\rangle = \sqrt{\frac{2}{3}}|F_-\rangle|R_+\rangle - \sqrt{\frac{1}{3}}|F_+\rangle|R_0\rangle, \quad (301)$$

$$|\Psi_{22,-}^{(0)}\rangle = \sqrt{\frac{1}{3}}|F_-\rangle|R_0\rangle - \sqrt{\frac{2}{3}}|F_+\rangle|R_-\rangle. \quad (302)$$

The occupations satisfy

$$(n_{c_+}, n_{d_+}; n_{c_-}, n_{d_-}) = (1, 1; 1, 1), \quad (N_+, N_-) = (2, 2). \quad (303)$$

Writing $\mathbf{R} = \mathbf{s}_{d_+} + \mathbf{s}_{d_-}$, the leading-order correlations are

$$\boxed{\begin{aligned} \langle \mathbf{s}_{d_+} \cdot \mathbf{s}_{d_-} \rangle_{22} &= \frac{1}{4}, \\ \langle \mathbf{F} \cdot \mathbf{R} \rangle_{22} &= -1, \\ \langle \mathbf{F} \cdot \mathbf{s}_{d_+} \rangle_{22} &= \langle \mathbf{F} \cdot \mathbf{s}_{d_-} \rangle_{22} = -\frac{1}{2}. \end{aligned}} \quad (304)$$

Thus both outer spins participate in the correlated ground state. The two outer spins align into a triplet, which couples antiferromagnetically to the central doublet. The center and the outer subsystem are entangled.

The closed-shell 31 and 13 states. If both outer electrons occupy d_+ , their state is

$$|D_+, 0_-\rangle = d_{+\uparrow}^\dagger d_{+\downarrow}^\dagger |0\rangle_{\text{out}}. \quad (305)$$

The resulting doublet is

$$\boxed{|\Psi_{31,\pm}^{(0)}\rangle = |F_\pm\rangle |D_+, 0_-\rangle}, \quad (306)$$

with

$$(n_{c_+}, n_{d_+}; n_{c_-}, n_{d_-}) = (1, 2; 1, 0), \quad (N_+, N_-) = (3, 1). \quad (307)$$

The channel-reversed configuration is

$$\boxed{|\Psi_{13,\pm}^{(0)}\rangle = |F_\pm\rangle |0_+, D_-\rangle}, \quad (308)$$

where

$$|0_+, D_-\rangle = d_{-\uparrow}^\dagger d_{-\downarrow}^\dagger |0\rangle_{\text{out}}. \quad (309)$$

Its occupations are $(1, 0; 1, 2)$, giving $(N_+, N_-) = (1, 3)$.

In either closed-shell configuration, the outer subsystem has zero spin:

$$\mathbf{s}_{d_+} |\text{CS}\rangle = \mathbf{s}_{d_-} |\text{CS}\rangle = 0. \quad (310)$$

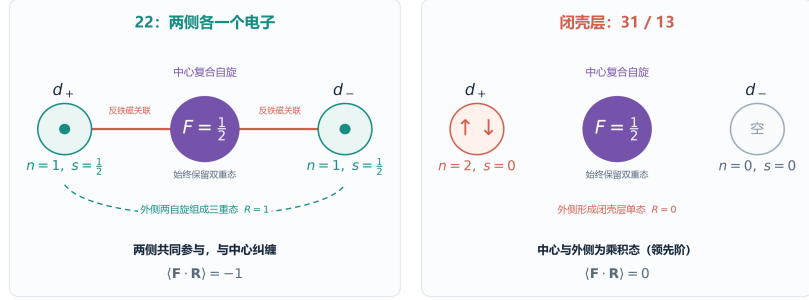
Consequently,

$$\langle \mathbf{F} \cdot \mathbf{R} \rangle_{CS} = 0, \quad \langle \mathbf{s}_{d+} \cdot \mathbf{s}_{d-} \rangle_{CS} = 0. \quad (311)$$

At this order, the central doublet and the outer closed shell form a product state. This does not imply that the impurity itself is uncorrelated: it remains entangled with the central electrons inside $|F_{\pm}\rangle$.

两个局域基态的差异

强交换极限 · 只画占据和自旋关联



两者的全体系总自旋都是 $1/2$ ；区别在外侧电子占据与关联。

右面画的是 $m > 0$ 的 31；d+ 双占据；交换两个轨道即为 13。

圆圈表示轨道或中心复合自旋；连线表示自旋关联，不表示跃迁。单电子箭头不指定自旋方向。

两类局域基态：三项 DMRG 观测量

$L = 32, N_e = 64, t = 1, J_A = J_B = J$; 周期边界; 8 个强耦合点均通过本批验收

中心—邻域关联 $B_3 = \langle (\mathbf{S}_d + \mathbf{S}_0^{\text{ring}}) \cdot (\mathbf{S}_{-1}^{\text{ring}} + \mathbf{S}_1^{\text{ring}}) \rangle$

左右横档关联 $C_{LR} = \langle \mathbf{S}_{-1}^{\text{ring}} \cdot \mathbf{S}_1^{\text{ring}} \rangle$

中心区域纠缠熵 $S_A = -\text{Tr}(\rho_A \ln \rho_A), \quad \mathcal{A} = \{A_0, \text{impurity}, B_0\}$

$\mathbf{S}_j^{\text{ring}} = \mathbf{S}_{jA} + \mathbf{S}_{jB}$; 0 为杂质横档; ± 1 为相邻横档; $\rho_A = \text{Tr}_{\mathcal{A}^c}(|\Psi\rangle\langle\Psi|)$.

α	J/t	ED 分支	B_3	C_{LR}	S_A (nats)
0	12	22	-0.617990	0.148993	1.719380
0	80	22	-0.959778	0.239916	0.836498
0.25	40	22	-0.875964	0.218783	1.111667
0.25	120	31	-9.0744×10^{-5}	7.3861×10^{-7}	0.043699
1	12	22	-0.553237	0.132567	1.728929
1	32	31	-0.001351	6.8302×10^{-5}	0.250971
2	8	22	-0.293907	0.055598	1.862949
2	20	31	-0.002784	1.3998×10^{-4}	0.296856

观测量全部来自原始晶格 DMRG; ED 仅用于能量基准及分支归属。均采用自然对数。

按 (N_+, N_-) 标记: $\alpha > 0$ 的闭壳层分支为 31; 交换通道名称后记为 13。 $\alpha = 0$ 两点均为 22。

31 代表点中，中心—邻域关联、左右关联及中心区域纠缠熵明显减弱。

这些是代表参数点的对照，不是密集相边界扫描；原始晶格关联含浴背景，未作背景扣除。

E Outlook.

One Determine the phase transition point $J(\alpha)$ with DMRG

Two Finding possible observables to explain $M(t)$ behaviour