# Supplemental Material: Correlation renormalized and induced spin-orbit coupling

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In this supplemental material, we provide the details of the Hartree-Fock mean field of multi-orbital Hubbard model $H_U$. Following six channels are decoupled

$$
\begin{aligned}
\hat{n}_{i,\alpha} &= \sum_{\sigma} \hat{n}^{\alpha\alpha}_{i,\sigma\sigma} \\
\hat{m}^{\mu}_{i,\alpha} &= \sum_{\sigma\sigma'} \sigma^{\mu}_{\sigma\sigma'} \hat{n}^{\alpha\alpha}_{i,\sigma\sigma} \\
\hat{L'}_{i,\alpha\beta} &= \sum_{\sigma} \hat{n}^{\alpha\beta}_{i,\sigma\sigma} (\alpha \neq \beta) \\
\hat{L''}_{i,\alpha\beta} &= \sum_{\sigma} \hat{n}^{\alpha\beta}_{i,\sigma\bar{\sigma}} (\alpha \neq \beta) \\
\hat{R'}_{i,\alpha\beta} &= \sum_{\sigma} \sigma \hat{n}^{\alpha\beta}_{i,\sigma\sigma} (\alpha \neq \beta) \\
\hat{R''}_{i,\alpha\beta} &= \sum_{\sigma} \sigma \hat{n}^{\alpha\beta}_{i,\sigma\bar{\sigma}} (\alpha \neq \beta) \\
\hat{n}^{\alpha\beta}_{i,\sigma\sigma'} &= C^{\dagger}_{i,\alpha\sigma} C_{i,\beta\sigma'}
\end{aligned}
\tag{1}
$$

Then, $H_U$ is decoupled as

$$
\begin{aligned}
H_U &= \sum_{i,\alpha} [\frac{U}{2} n_{i,\alpha} + (U' - \frac{J}{2}) \sum_{\alpha\neq\beta} n_{i,\beta}] \hat{n}_{i,\alpha} \\
&- \sum_{i,\alpha\mu} [\frac{U}{2} m^{\mu}_{i,\alpha} + \frac{J}{2} \sum_{\alpha\neq\beta} m^{\mu}_{i,\beta}] \hat{m}^{\mu}_{i,\alpha} \\
&+ \sum_{i,\alpha\neq\beta} [(-\frac{U'}{2} + J) L'_{i,\beta\alpha} + \frac{J}{2} L'_{i,\alpha\beta}] \hat{L'}_{i,\alpha\beta} \\
&- \sum_{i,\alpha\neq\beta} [\frac{U'}{2} L''_{i,\beta\alpha} + \frac{J}{2} L''_{i,\alpha\beta}] \hat{L''}_{i,\alpha\beta} \\
&- \sum_{i,\alpha\neq\beta} [\frac{U'}{2} R'_{i,\beta\alpha} + \frac{J}{2} R'_{i,\alpha\beta}] \hat{R'}_{i,\alpha\beta} \\
&+ \sum_{i,\alpha\neq\beta} [\frac{U'}{2} R''_{i,\beta\alpha} + \frac{J}{2} R''_{i,\alpha\beta}] \hat{R''}_{i,\alpha\beta} + const.
\end{aligned}
\tag{2}
$$

To understand general mean-field orders, for N general orbits, all the general orbital orders are represent as $N*N$ Hermitian matrices.

$$
< O_{\alpha\beta} >=< \eta C^{\dagger}_{\alpha} C_{\beta} + \eta^{*} C^{\dagger}_{\beta} C_{\alpha} > \tag{3}
$$

where $\eta$ is coefficient.

$N*N$ Hermitian matrices can be decomposed using SU(N) generators and identity matrix. SU(N) Lie algebra contains $N^2-1$ generators, or named orbital isospin operators. We always choose three types of matrices as extension Pauli matrices in SU(2). In defining representation, symmetric non-diagonal $\sigma_x$ is extended to $T^{(1)}_{\alpha\beta}$ and its matrix as

$$
(T^{(1)}_{\alpha\beta})_{ab} = \frac{1}{2} (\delta_{\alpha a}\delta_{\beta b} + \delta_{\beta a}\delta_{\alpha b}) \ (\alpha < \beta) \tag{4}
$$

where $\alpha/\beta$ are labels for generators and $a, b$ are matrices indices. All of them are ranging 1 to N.

And anti-symmetry $\sigma_y$ is extended as $T^{(2)}_{\alpha\beta}$

$$
(T^{(2)}_{\alpha\beta})_{ab} = \frac{-i}{2} (\delta_{\alpha a}\delta_{\beta b} - \delta_{\beta a}\delta_{\alpha b}) \ (\alpha < \beta) \tag{5}
$$

The third traceless diagonal $\sigma_z$ is extended as $T^{(3)}_{\alpha} (\alpha > 1)$ and normalized as

$$
(T^{(3)}_{\alpha})_{ab} = \begin{cases} \delta_{ab}(2\alpha(\alpha-1))^{-1/2}, & \text{if } a < \alpha, \\ -\delta_{ab}(\frac{(\alpha-1)}{2\alpha})^{-1/2}, & \text{if } a = \alpha, \\ 0, & \text{if } a > \alpha \end{cases} \tag{6}
$$

We have $\frac{N(N-1)}{2}$ symmetric $T^{(1)}_{\alpha\beta}$, anti-symmetric $\frac{N(N-1)}{2}$ $T^{(2)}_{\alpha\beta}$ and traceless $N-1$ $T^{(3)}_{\alpha}$ with total number of generators $N^2-1$. Including identity labeled $T^3_1$, we have full $N^2$ basis for $N*N$ matrices.

Taking $SU(3)$ for example, $T^{(1)}_{\alpha\beta}$ are

$$
T^{(1)}_{12} = \frac{\lambda_1}{2} = \frac{1}{2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{7}
$$

$$
T^{(1)}_{13} = \frac{\lambda_4}{2} = \frac{1}{2} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \tag{8}
$$

$$
T^{(1)}_{23} = \frac{\lambda_6}{2} = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{9}
$$

$T^{(2)}_{\alpha\beta}$ are

$$T^{(2)}_{12} = \frac{\lambda_2}{2} = \frac{1}{2}\begin{bmatrix}0 & -i & 0\\ i & 0 & 0\\ 0 & 0 & 0\end{bmatrix} \quad (10)$$

$$T^{(2)}_{13} = \frac{\lambda_5}{2} = \frac{1}{2}\begin{bmatrix}0 & 0 & -i\\ 0 & 0 & 0\\ i & 0 & 0\end{bmatrix} \quad (11)$$

$$T^{(2)}_{23} = \frac{\lambda_7}{2} = \frac{1}{2}\begin{bmatrix}0 & 0 & 0\\ 0 & 0 & -i\\ 0 & i & 0\end{bmatrix} \quad (12)$$

$T^{(3)}_{\alpha}$ are

$$T^{(3)}_{2} = \frac{\lambda_3}{2} = \frac{1}{2}\begin{bmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 0\end{bmatrix} \quad (13)$$

$$T^{(3)}_{3} = \frac{\lambda_8}{2} = \frac{1}{2\sqrt{3}}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -2\end{bmatrix} \quad (14)$$

where $\lambda_i$ are well-known Gell-Mann matrices for $SU(3)$.

For diagonal orders, identity $T^{(3)}_1$ is total density. And other $T^{(3)}_\alpha$ are ferro-orbital orders and crystal field for $\alpha$ and $\beta$ orbits. Typically, crystal field is diagonal and ferro-orbital for different crystal field class. For example, $t_{2g}$ are more occupied than $e_g$ orbitals in octahedral environment.

For symmetric $T^{(1)}_{\alpha\beta}$, orders are represent as

$$< T^{(1)}_{\alpha\beta} >= \frac{1}{2} < C^\dagger_\alpha C_\beta + C^\dagger_\beta C_\alpha > \quad (15)$$

$T^{(1)}_{\alpha\beta}$ are off-diagonal density matrix for correlated orbitals defined in LDA+U, which are also named on-site interorbial single-electron hopping.

For ani-symmetric $T^{(2)}_{\alpha\beta}$, orders are represent as

$$< T^{(2)}_{\alpha\beta} >= \frac{i}{2} < C^\dagger_\alpha C_\beta - C^\dagger_\beta C_\alpha > \quad (16)$$

Using real orbits, orbital angular momentum $L_i$ are always complex and anti-symmetry as in $T^{(2)}_{\alpha\beta}$. Angular momentums $L_i$ are well defined in SO(3) symmetric systems. For general lattices, $L_i$ are not defined. Thus, we extend 3 $L_i$ in 3D to generalized $\frac{N(N-1)}{2}$ orbital angular momentum $T^{(2)}_{\alpha\beta}$. For $N > 3$, there are more than 3 angular momentums. Angular momentums are expanded as

$$L_i = \sum_{\alpha\beta} l^i_{\alpha\beta} T^{(2)}_{\alpha\beta} \quad (17)$$

$l^i_{\alpha\beta}$ are coefficients of $L_i$.

In general, local Fermionic Hilbert space is spanned by orbital and spin tensor space. Spin order is defined as Pauli matrices $\sigma_i$ in SU(2). For charge order including ferro-orbital orders, with number N-1 (1 for total charge)

$$\hat{n}_\alpha = \sum_\beta n_{\alpha\beta} T^{(3)}_\beta \otimes \sigma_0 \quad (18)$$

For general spin order, with number 3N

$$\hat{m}^\mu_\alpha = \sum_\beta m_{\alpha\beta} T^{(3)}_\beta \otimes \sigma_\mu \quad (19)$$

Then we have general symmetric orbital orders, with number $\frac{N(N-1)}{2}$

$$\hat{O}_{\alpha\beta} = T^{(1)}_{\alpha\beta} \otimes \sigma_0 \quad (20)$$

Generalized anti-symmetric angular momentum orders, with number $\frac{N(N-1)}{2}$

$$\hat{L}_{\alpha\beta} = T^{(2)}_{\alpha\beta} \otimes \sigma_0 \quad (21)$$

Orbital order with spin order, with number $\frac{3N(N-1)}{2}$

$$\hat{OS}^\mu_{\alpha\beta} = T^{(1)}_{\alpha\beta} \otimes \sigma_\mu \quad (22)$$

Generalized spin-orbital coupling, with number $\frac{3N(N-1)}{2}$

$$\hat{LS}^\mu_{\alpha\beta} = T^{(2)}_{\alpha\beta} \otimes \sigma_\mu \quad (23)$$

The relations between order defined here and $\hat{L}'$,$\hat{L}''$, $\hat{R}'$,$\hat{R}''$.

$$\begin{aligned}
Re(\hat{L}'_{\alpha\beta}) &= \hat{O}_{\alpha\beta} \propto U' - 3J & (24)\\
Im(\hat{L}'_{\alpha\beta}) &= \hat{L}_{\alpha\beta} \propto U' - J & (25)\\
Re(\hat{R}'_{\alpha\beta}) &= \hat{OS}^z_{\alpha\beta} \propto U' + J & (26)\\
Im(\hat{R}'_{\alpha\beta}) &= \hat{LS}^z_{\alpha\beta} \propto U' - J & (27)\\
Re(\hat{L}''_{\alpha\beta}) &= \hat{OS}^x_{\alpha\beta} \propto U' + J & (28)\\
Im(\hat{L}''_{\alpha\beta}) &= \hat{LS}^x_{\alpha\beta} \propto U' - J & (29)\\
Re(\hat{R}''_{\alpha\beta}) &= \hat{LS}^y_{\alpha\beta} \propto U' + J & (30)\\
Im(\hat{R}''_{\alpha\beta}) &= \hat{OS}^y_{\alpha\beta} \propto U' - J & (31)
\end{aligned}$$

$Re$ and $Im$ are real and imaginary parts.

The total number of orders for $2N \times 2N$ matrix are

$$N - 1 + 3N + N(N-1) + 3N(N-1) = 4N^2 - 1 \quad (32)$$

**RG part**

To to RG, we first need expand around the QBCP with effective continuous model. To keep QBCP, $t_\pi < 0$. When $t_\pi = 0$, there are two exact flat bands. And when $t_\pi > 0$, there are no QBCP anymore without any instability. The low energy effective model is described

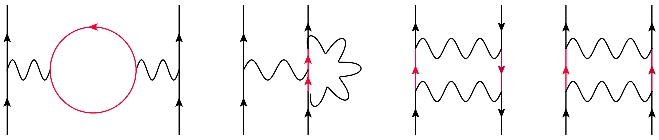

FIG. 1: Four types of one-loop Feynman diagram included in our RG calculations. The red lines are loops integrated.

by $\psi_{p_{x/y},\sigma} = \frac{1}{\sqrt{2}}(\psi_{\sigma,A,p_{x/y}} + \psi_{\sigma,B,p_{x/y}})$. Under this basis transformation, interaction vertices remain same form as in multi-orbital hubbard model.

$$H_{QBC}(k) = \frac{t_\sigma + t_\pi}{2}k^2\sigma_0 + \frac{t_\sigma - t_\pi}{4}(k^2\sigma_z + \sqrt{3}(k_x^2 - k_y^2)\sigma_x) = d_0\sigma_0 + d_x\sigma_x + d_z\sigma_z \quad (33)$$

The non-interacting Green's function $(G_0^\sigma(\omega, \mathbf{k}))^{-1} = (i\omega - d_0)\sigma_0 - d_x\sigma_x - d_z\sigma_z$. Then, we integrate out fast modes between cutoff $\Lambda$ and $\frac{\Lambda}{s}$.We have four interaction vertices and perform one-loop RG including four types of Feynman diagrams. The essentail fermion loop integrals are listed below:

$$ZS1 : \int_k G^\sigma_{0aa}(k)G^{\sigma'}_{0\bar{a}\bar{a}}(k) = -\eta dl \quad (34)$$

$$ZS2 : \int_k G^\sigma_{0a\bar{a}}(k)G^{\sigma}_{0\bar{a}a}(k) = \gamma dl \quad (35)$$

$$ZS3 : \int_k G^\sigma_{0aa}(k)G^{\sigma'}_{0aa}(k) = -\gamma dl \quad (36)$$

$$BCS1 : \int_k G^\sigma_{0aa}(k)G^{\sigma'}_{0\bar{a}\bar{a}}(-k) = \gamma dl \quad (37)$$

$$BCS2 : \int_k G^\sigma_{0a\bar{a}}(k)G^{\sigma'}_{0\bar{a}a}(-k) = \gamma dl \quad (38)$$

$$BCS3 : \int_k G^\sigma_{0aa}(k)G^{-\sigma'}_{0aa}(-k) = \eta dl \quad (39)$$

where $\int_k = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\int_0^{2\pi}\frac{d\theta}{2\pi}\int_{\frac{\Lambda}{s}}^{\Lambda}\frac{dk}{2\pi}$ and $s = e^{dl}$. To more precisely,

$$\eta = \int_0^{2\pi} d\theta \frac{f_x^2(\theta) + 2f_z^2(\theta)}{4(f_x^2(\theta) + f_z^2(\theta))^{\frac{3}{2}}} \quad (40)$$

$$\gamma = \int_0^{2\pi} d\theta \frac{f_x^2(\theta)}{4(f_x^2(\theta) + f_z^2(\theta))^{\frac{3}{2}}} \quad (41)$$

$$f_x(\theta) = \frac{\sqrt{3}}{4}(t_\sigma - t_\pi)(\cos\theta^2 - \sin\theta^2) \quad (42)$$

$$f_z(\theta) = \frac{1}{4}(t_\sigma - t_\pi)(\cos\theta^2 + \sin\theta^2) \quad (43)$$

In Figs.2-5, we list all one-loop Feynman diagrams contributing to interaction renormalization.

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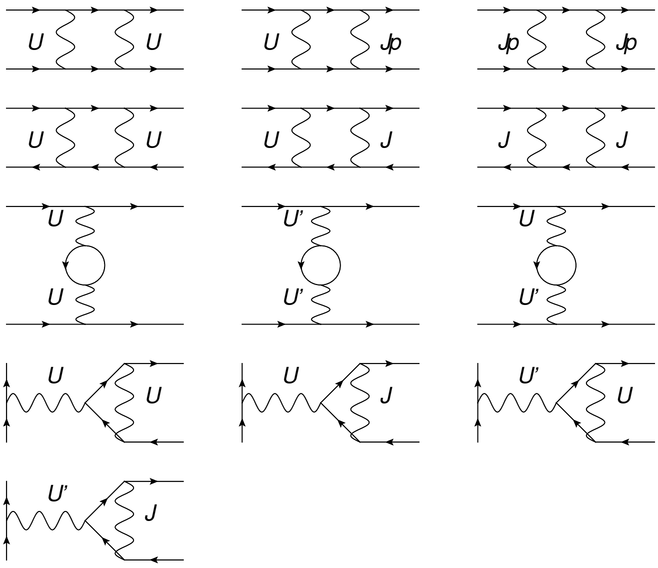


FIG. 2: Feynman diagrams contributing to $U$ renormalization.

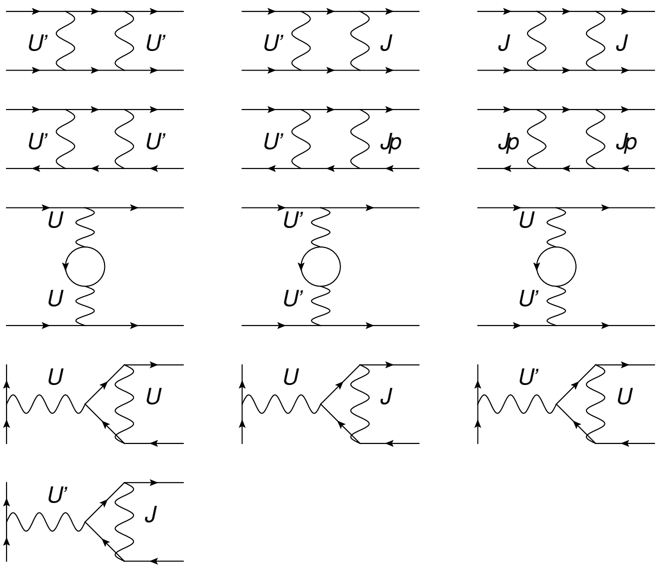


FIG. 3: Feynman diagrams contributing to $U'$ renormalization.

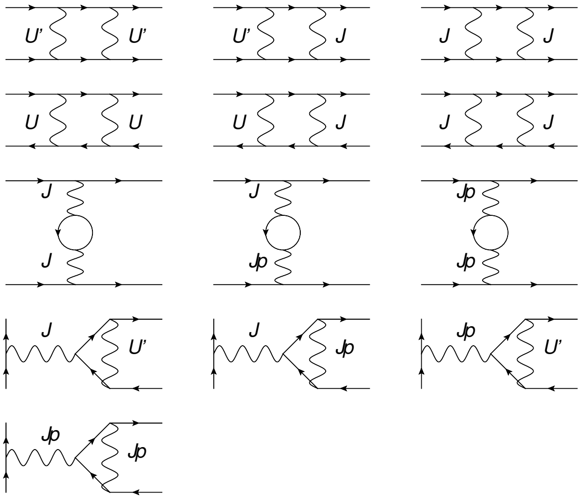


FIG. 4: Feynman diagrams contributing to $J$ renormalization.

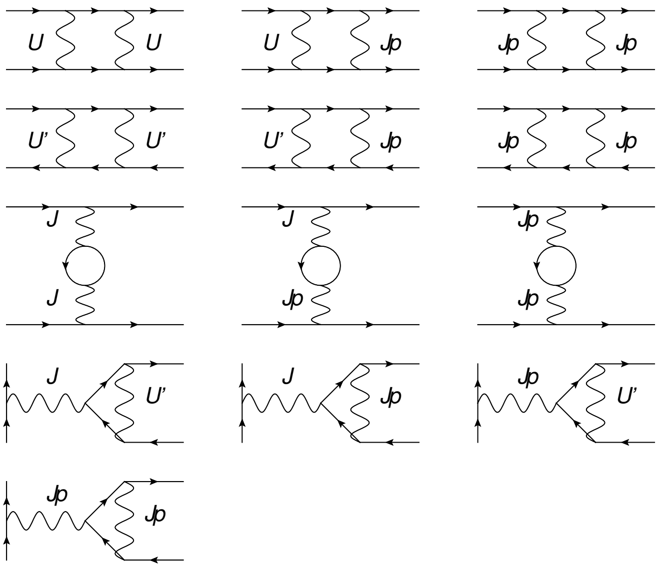


FIG. 5: Feynman diagrams contributing to $J_p$ renormalization.