Supplementary Material: Magnetism and Superconductivity in the $t-J$ Model of $La_3Ni_2O_7$ Under Multiband Gutzwiller Approximation

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I. DETAILS ON THE $t-J$ MODEL

We constrain the Hilbert space to consist of five states at each site and perform the standard second-order perturbation theory, the superexchange coupling parameters are related to the original parameters through the following equations:

$$
\begin{aligned}
J_1 &= \frac{4(t_{11}^{\text{intra}})^2}{U_1} + \frac{2(t_{12}^{\text{intra}})^2}{J_H + U' + \epsilon_2}\,, \\
J_2 &= \frac{4(t_{11}^{\text{inter}})^2}{U_1}\,, \\
J_1' &= 2(t_{11}^{\text{intra}})^2\left(\frac{1}{U_1+U'} + \frac{1}{U_1-U'+J_H}\right) \\
&\quad + 2(t_{12}^{\text{intra}})^2\left(\frac{1}{U_2+U'+\epsilon_2} + \frac{1}{U_1-U'-\epsilon_2+J_H}\right) \\
&\quad + (t_{12}^{\text{intra}})^2\left(\frac{1}{2J_H+\epsilon_2} - \frac{1}{\epsilon_2}\right) + \frac{(t_{22}^{\text{intra}})^2}{2J_H}\,, \\
J_2' &= 2(t_{11}^{\text{inter}})^2\left(\frac{1}{U_1+U'} + \frac{1}{U_1-U'+J_H}\right) + \frac{(t_{22}^{\text{inter}})^2}{2J_H}\,, \\
J_{d1} &= \frac{(t_{11}^{\text{intra}})^2}{U_1+J_H} + \frac{(t_{22}^{\text{intra}})^2}{U_2+J_H} \\
&\quad + (t_{12}^{\text{intra}})^2\left(\frac{1}{U_1+J_H-\epsilon_2} + \frac{1}{U_2+J_H+\epsilon_2}\right), \\
J_{d2} &= \frac{(t_{11}^{\text{inter}})^2}{U_1+J_H} + \frac{(t_{22}^{\text{inter}})^2}{U_2+J_H}\,,
\end{aligned}
\tag{1}
$$

where the third term $(t_{12}^{\text{intra}})^2(\frac{1}{2J_H+\epsilon_2} - \frac{1}{\epsilon_2})$ in J_1' is from the superexchange process between the half-filled and empty orbitals, and contributes to the intra-layer ferromagnetic coupling, which is absent in J_2' since the inter-orbital hopping between layers is zero.

II. DERIVATION OF THE SELF-CONSISTENT MEAN-FIELD HAMILTONIAN

In the main text, we define the Gutzwiller projection operator $\hat{P}$, which is expressed in terms of fugacities η and operators $\hat{Q}$. To be specific, operators $\hat{Q}$ are defined as:

$$
\begin{aligned}
\hat{Q}_{1e,\sigma}(il) &= \hat{n}_{1l;i\sigma}(1-\hat{n}_{1l;i\bar{\sigma}})(1-\hat{n}_{2l;i\uparrow})(1-\hat{n}_{2l;i\downarrow})\,, \\
\hat{Q}_{2e,\sigma\sigma'}(il) &= \hat{n}_{1l;i\sigma}(1-\hat{n}_{1l;i\bar{\sigma}})\hat{n}_{2l;i\sigma'}(1-\hat{n}_{2l;i\bar{\sigma}'})\,,
\end{aligned}
\tag{2}
$$

and the fugacities η are related to the expections of operators $\hat{Q}$ through:

$$
\begin{aligned}
\langle \hat{Q}_{1e,\sigma}(il)\rangle &= \frac{\langle \hat{P}\hat{Q}_{1e,\sigma}(il)\hat{P}\rangle_0}{\langle \hat{P}\hat{P}\rangle_0} \\
&= \frac{\langle \prod_{jl'\neq il}\hat{P}^2(jl')\hat{P}(il)\hat{Q}_{1e,\sigma}(il)\hat{P}(il)\rangle_0}{\prod_{il} z_{il}} \\
&= \frac{\eta_{1\sigma}^2(il)\langle \hat{Q}_{1e,\sigma}(il)\rangle_0}{z_{il}}\,,
\end{aligned}
\tag{3}
$$

where $z_{il} = \langle \hat{P}^2(il)\rangle_0$. It is also easy to see that $\eta^2_{2\sigma\sigma'}(il)/z_{il} = \langle \hat{Q}_{2e,\sigma\sigma'}(il)\rangle / \langle \hat{Q}_{2e,\sigma\sigma'}(il)\rangle_0$. we further make approximations about the expectation of operators $\hat{Q}$ before and after the projection, so that:

$$\begin{aligned}
&\langle \hat{Q}_{1e,\sigma}(il)\rangle = \delta\, n_{1l;i\sigma}\,,\\
&\langle \hat{Q}_{2e,\sigma\sigma'}(il)\rangle = n_{1l;i\sigma} n_{2l;i\sigma'}\,,\\
&\langle \hat{Q}_{1e,\sigma}(il)\rangle_0 = n^0_{1l;i\sigma}(1-n^0_{1l;i\bar{\sigma}})(1-n^0_{2l;i\uparrow})(1-n^0_{2l;i\downarrow})\,,\\
&\langle \hat{Q}_{2e,\sigma\sigma'}(il)\rangle_0 = n^0_{1l;i\sigma}(1-n^0_{1l;i\bar{\sigma}}) n^0_{2l;i\sigma'}(1-n^0_{2l;i\bar{\sigma}'})\,.
\end{aligned} \tag{4}$$

Where δ is the hole doping parameter. Here, we assume the electron densities before and after projection are same, that is $n_{\alpha l;i\sigma} = n^0_{\alpha l;i\sigma}$. With these relations, we can evaluate the energy $E = \langle \hat{H}_{t-J}\rangle$. By taking Wick contractions, the energy E can be express in terms of expectation values with respect to the non-interacting state $|\psi_0\rangle$. Here we take one kinetic term as an example to illustrate the process.

$$\begin{aligned}
&\langle c^\dagger_{2l;i\sigma} c_{2l;j\sigma}\rangle\\
&= \frac{\langle \hat{P}(il) c^\dagger_{2l;i\sigma} \hat{P}(il) \hat{P}(jl) c_{2l;j\sigma} \hat{P}(jl)\rangle_0}{z_{il} z_{jl}}\\
&= \frac{1}{z_{il} z_{jl}} [\eta_{1\sigma}(il)\eta_{2\sigma\sigma}(il)\eta_{1\sigma}(jl)\eta_{2\sigma\sigma}(jl) \langle \hat{Q}_{2e,\sigma\sigma}(il) c^\dagger_{2l;i\sigma} \hat{Q}_{1e,\sigma}(il) \hat{Q}_{1e,\sigma}(jl) c_{2l;j\sigma} \hat{Q}_{2e,\sigma\sigma}(jl)\rangle_0\\
&\quad + \cdots]\,.
\end{aligned} \tag{5}$$

Considering the Hamiltonian is defined in the restricted Hilbert space, the operator $c^\dagger_{2l;i\sigma}$ should be understanded as $c^\dagger_{2l;i\sigma} \equiv \hat{P}_{triplet}(il) c^\dagger_{2l;i\sigma}$, with $\hat{P}_{triplet}(il) = (\boldsymbol{S}_{1l;i}\cdot \boldsymbol{S}_{2l;i} + \frac{3}{4})$ projecting out the spin-singlet state. Similarly $c_{2l;j\sigma} \equiv c_{2l;j\sigma} \hat{P}_{triplet}(jl)$. We substitute (2) into equation (5), the first term in (5) is then:

$$\begin{aligned}
&\langle \hat{Q}_{2e,\sigma\sigma}(il) c^\dagger_{2l;i\sigma} \hat{Q}_{1e,\sigma}(il) \hat{Q}_{1e,\sigma}(jl) c_{2l;j\sigma} \hat{Q}_{2e,\sigma\sigma}(jl)\rangle_0\\
&= -\langle c^\dagger_{1l;i\sigma} c^\dagger_{1l;j\sigma} c^\dagger_{2l;i\sigma} c_{1l;i\sigma} c_{1l;j\sigma} c_{2l;j\sigma}\rangle_0 + \ldots\\
&= n_{1l;i\sigma} n_{1l;j\sigma} \chi^{\text{intra}}_{(2l;i\sigma)(2l;j\sigma)} - \chi^{\text{intra}}_{(1l;i\sigma)(1l;j\sigma)} \chi^{\text{intra}}_{(1l;j\sigma)(1l;i\sigma)} \chi^{\text{intra}}_{(2l;i\sigma)(2l;j\sigma)}\\
&\quad + \chi^{\text{intra}}_{(1l;i\sigma)(2l;j\sigma)} \chi^{\text{intra}}_{(1l;j\sigma)(1l;i\sigma)} \chi^{\text{intra}}_{(2l;i\sigma)(1l;j\sigma)} + \cdots\,.
\end{aligned} \tag{6}$$

After evaluating the J-term as was done for the kinetic term above, we finally get the total energy $E = E(\chi, \Delta, n)$ which is expressed in terms of non-interacting expectations. In this work, we don't relate the expectations after projection to the expectations before projection by a simple multiplicative factor, like $\langle c^\dagger_{2l;i\sigma} c_{2l;j\sigma}\rangle = g_t \langle c^\dagger_{2l;i\sigma} c_{2l;j\sigma}\rangle_0$, instead, we include the inter-site correlation and take all possible Wick contractions to derive a relatively complicated expression for the energy. We believe that this is a better choice to deal with the strong correlated materials.

III. CALCULATION OF THE SUPERFLUID STIFFNESS

With the self-consistent numerical results of the mean-field Hamiltonian, it is straighforward to evaluate the equation for superfluid stiffness presented in the main text. Substituting equation (9) into (8), the resulting current-current correlation function can be expressed as:

$$\begin{aligned}
&\Lambda_{xx}(\mathbf{q}, i\omega_n)\\
&= C\int_0^\beta d\tau e^{i\omega_n\tau} \sum_{\substack{ll'\sigma\sigma'\mathbf{k}\mathbf{k}'\\ \alpha\neq\beta,\gamma\neq\delta}} \sin\left(\frac{k_x + \frac{q_x}{2}}{\sqrt{2}}\right) \sin\left(\frac{k'_x - \frac{q_x}{2}}{\sqrt{2}}\right) \langle c^\dagger_{2l;\alpha\sigma}(\mathbf{k}+\mathbf{q},\tau) c_{2l;\beta\sigma}(\mathbf{k},\tau) c^\dagger_{2l';\gamma\sigma'}(\mathbf{k'}-\mathbf{q},0) c_{2l',\delta\sigma'}(\mathbf{k}',0)\rangle\\
&= Cg^2\int_0^\beta d\tau e^{i\omega_n\tau} \sum_{\substack{ll'\sigma\sigma'\mathbf{k}\mathbf{k}'\\ \alpha\neq\beta,\gamma\neq\delta}} \sin\left(\frac{k_x + \frac{q_x}{2}}{\sqrt{2}}\right) \sin\left(\frac{k'_x - \frac{q_x}{2}}{\sqrt{2}}\right) (A+B)\,,
\end{aligned} \tag{7}$$

where $C = 2(t^{\text{intra}}_{22})^2/N$, and the elements A and B are given by:

$$A = -\langle c^\dagger_{2l;\alpha\sigma}(\mathbf{k}+\mathbf{q},\tau) c^\dagger_{2l';\gamma\sigma'}(\mathbf{k'}-\mathbf{q},0)\rangle_0 \langle c_{2l;\beta\sigma}(\mathbf{k},\tau) c_{2l',\delta\sigma'}(\mathbf{k}',0)\rangle_0\,, \tag{8}$$

$$B = \langle c^\dagger_{2l;\alpha\sigma}(\mathbf{k}+\mathbf{q},\tau) c_{2l',\delta\sigma'}(\mathbf{k}',0)\rangle_0 \langle c_{2l;\beta\sigma}(\mathbf{k},\tau) c^\dagger_{2l';\gamma\sigma'}(\mathbf{k'}-\mathbf{q},0)\rangle_0\,. \tag{9}$$

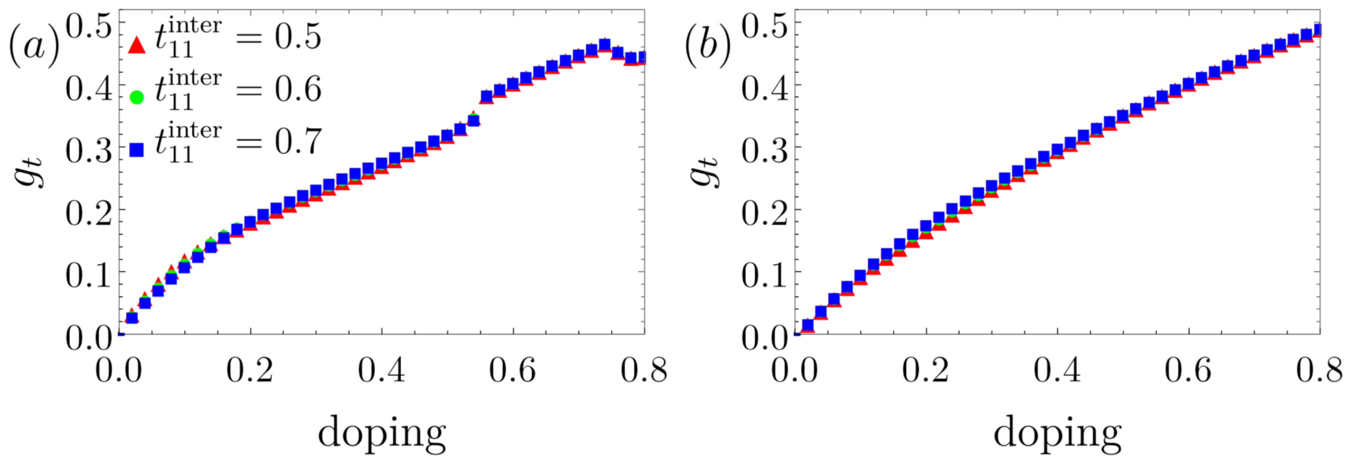

FIG. 1. The renormalized factor g versus hole doping for superconducting phases (a) with and (b) without G-AFM order.

In the last step of equation (7), we apply Wick's theorem. Using the unitary matrix $U(\mathbf{k})$ which diagonalizes the effective mean-field Hamiltonian in momentum space with the basis operator $\Psi^{\dagger}_{Sl;\alpha\sigma}(\mathbf{k}) = [c^{\dagger}_{1t;A\uparrow}(\mathbf{k}), c^{\dagger}_{1t;B\uparrow}(\mathbf{k}), c^{\dagger}_{2t;A\uparrow}(\mathbf{k}), c^{\dagger}_{2t;B\uparrow}(\mathbf{k}), c^{\dagger}_{1b;A\uparrow}(\mathbf{k}), c^{\dagger}_{1b;B\uparrow}(\mathbf{k}), c^{\dagger}_{2b;A\uparrow}(\mathbf{k}), c^{\dagger}_{2b;B\uparrow}(\mathbf{k}), c_{1t;A\downarrow}(-\mathbf{k}), c_{1t;B\downarrow}(-\mathbf{k}), c_{2t;A\downarrow}(-\mathbf{k}), c_{2t;B\downarrow}(-\mathbf{k}), c_{1b;A\downarrow}(-\mathbf{k}), c_{1b;B\downarrow}(-\mathbf{k}), c_{2b;A\downarrow}(-\mathbf{k}), c_{2b;B\downarrow}(-\mathbf{k})]$, the correlators in the above equation can be further expressed as:

$$\begin{aligned}
&\sum_{\sigma\sigma'}\langle c^{\dagger}_{2l;\alpha\sigma}(\mathbf{k}+\mathbf{q},\tau)c^{\dagger}_{2l';\gamma\sigma'}(\mathbf{k}'-\mathbf{q},0)\rangle_0\langle c_{2l;\beta\sigma}(\mathbf{k},\tau)c_{2l',\delta\sigma'}(\mathbf{k}',0)\rangle_0\\
&= -\delta_{\mathbf{k}',-\mathbf{k}}\sum_{n,m}U^{\dagger n}_{(2l;\alpha\uparrow)}(\mathbf{k}+\mathbf{q})U^{(2l';\gamma\downarrow)}_{n}(\mathbf{k}+\mathbf{q})U^{\dagger m}_{(2l';\delta\downarrow)}(\mathbf{k})U^{(2l;\beta\uparrow)}_{m}(\mathbf{k})\langle\tilde{c}^{\dagger}_{n\mathbf{k}+\mathbf{q}}(\tau)\tilde{c}_{n\mathbf{k}+\mathbf{q}}(0)\rangle_0\langle\tilde{c}^{\dagger}_{m\mathbf{k}}(0)\tilde{c}_{m\mathbf{k}}(\tau)\rangle_0\\
&\quad+U^{\dagger n}_{(2l';\gamma\uparrow)}(\mathbf{k}'-\mathbf{q})U^{(2l;\alpha\downarrow)}_{n}(\mathbf{k}'-\mathbf{q})U^{\dagger m}_{(2l;\beta\downarrow)}(\mathbf{k}')U^{(2l';\delta\uparrow)}_{m}(\mathbf{k}')\langle\tilde{c}^{\dagger}_{n\mathbf{k}'-\mathbf{q}}(0)\tilde{c}_{n\mathbf{k}'-\mathbf{q}}(\tau)\rangle_0\langle\tilde{c}^{\dagger}_{m\mathbf{k}'}(\tau)\tilde{c}_{m\mathbf{k}'}(0)\rangle_0\,,\\
&\sum_{\sigma\sigma'}\langle c^{\dagger}_{2l;\alpha\sigma}(\mathbf{k}+\mathbf{q},\tau)c_{2l';\delta\sigma'}(\mathbf{k}',0)\rangle_0\langle c_{2l;\beta\sigma}(\mathbf{k},\tau)c^{\dagger}_{2l',\gamma\sigma'}(\mathbf{k}'-\mathbf{q},0)\rangle_0\\
&= -\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\sum_{n,m}U^{\dagger n}_{(2l;\alpha\uparrow)}(\mathbf{k}+\mathbf{q})U^{(2l';\delta\uparrow)}_{n}(\mathbf{k}+\mathbf{q})U^{\dagger m}_{(2l';\gamma\uparrow)}(\mathbf{k})U^{(2l;\beta\uparrow)}_{m}(\mathbf{k})\langle\tilde{c}^{\dagger}_{n\mathbf{k}+\mathbf{q}}(\tau)\tilde{c}_{n\mathbf{k}+\mathbf{q}}(0)\rangle_0\langle\tilde{c}^{\dagger}_{m\mathbf{k}}(0)\tilde{c}_{m\mathbf{k}}(\tau)\rangle_0\\
&\quad+U^{\dagger n}_{(2l';\delta\downarrow)}(-\mathbf{k}')U^{(2l;\alpha\downarrow)}_{n}(-\mathbf{k}')U^{\dagger m}_{(2l;\beta\downarrow)}(-\mathbf{k}'+\mathbf{q})U^{(2l';\gamma\downarrow)}_{m}(-\mathbf{k}'+\mathbf{q})\langle\tilde{c}^{\dagger}_{n-\mathbf{k}'}(0)\tilde{c}_{n-\mathbf{k}'}(\tau)\rangle_0\langle\tilde{c}^{\dagger}_{m-\mathbf{k}'+\mathbf{q}}(\tau)\tilde{c}_{m-\mathbf{k}'+\mathbf{q}}(0)\rangle_0\,,
\end{aligned} \tag{10}$$

where $\tilde{c}^{\dagger}_{n\mathbf{k}}$ are defined as $\tilde{c}^{\dagger}_{n\mathbf{k}} = c^{\dagger}_{Sl;\alpha\sigma}(\mathbf{k})U^{(Sl;\alpha\sigma)}_{n}(\mathbf{k})$. Considering:

$$\begin{aligned}
\langle\tilde{c}^{\dagger}_{n\mathbf{k}}(\tau)\tilde{c}_{n\mathbf{k}}(0)\rangle_0 &= e^{E_n(\mathbf{k})\tau}n_F(E_n(\mathbf{k}))\,,\\
\langle\tilde{c}^{\dagger}_{n\mathbf{k}}(0)\tilde{c}_{n\mathbf{k}}(\tau)\rangle_0 &= -(1-n_F(E_n(\mathbf{k})))e^{-E_n(\mathbf{k})\tau}\,.
\end{aligned} \tag{11}$$

With these relations, we finally have:

$$
\begin{aligned}
&\Lambda_{xx}(\mathbf{q}, i\omega_n) \\
&= Cg^2 \sum_{\substack{ll'\mathbf{k}nm \\ \alpha\neq\beta,\gamma\neq\delta}} [-\sin\left(\frac{k_x+\frac{q_x}{2}}{\sqrt{2}}\right)^2 U^{\dagger n}_{(2l;\alpha\uparrow)}(\mathbf{k}+\mathbf{q}) U_n^{(2l';\gamma\downarrow)}(\mathbf{k}+\mathbf{q}) U^{\dagger m}_{2l';\delta\downarrow}(\mathbf{k}) U_m^{(2l;\beta\uparrow)}(\mathbf{k}) \frac{n_F(E_n(\mathbf{k}+\mathbf{q}))-n_F(E_m(\mathbf{k}))}{i\omega_n+E_n(\mathbf{k}+\mathbf{q})-E_m(\mathbf{k})} \\
&\quad -\sin\left(\frac{k_x-\frac{q_x}{2}}{\sqrt{2}}\right)^2 U^{\dagger n}_{(2l';\gamma\uparrow)}(\mathbf{k}-\mathbf{q}) U_n^{(2l;\alpha\downarrow)}(\mathbf{k}-\mathbf{q}) U^{\dagger m}_{2l;\beta\downarrow}(\mathbf{k}) U_m^{(2l';\delta\uparrow)}(\mathbf{k}) \frac{n_F(E_m(\mathbf{k}))-n_F(E_n(\mathbf{k}-\mathbf{q}))}{i\omega_n+E_m(\mathbf{k})-E_n(\mathbf{k}-\mathbf{q})} \\
&\quad -\sin\left(\frac{k_x+\frac{q_x}{2}}{\sqrt{2}}\right)^2 U^{\dagger n}_{(2l;\alpha\uparrow)}(\mathbf{k}+\mathbf{q}) U_n^{(2l';\delta\uparrow)}(\mathbf{k}+\mathbf{q}) U^{\dagger m}_{2l';\gamma\uparrow}(\mathbf{k}) U_m^{(2l;\beta\uparrow)}(\mathbf{k}) \frac{n_F(E_n(\mathbf{k}+\mathbf{q}))-n_F(E_m(\mathbf{k}))}{i\omega_n+E_n(\mathbf{k}+\mathbf{q})-E_m(\mathbf{k})} \\
&\quad -\sin\left(\frac{k_x-\frac{q_x}{2}}{\sqrt{2}}\right)^2 U^{\dagger n}_{(2l';\delta\downarrow)}(-\mathbf{k}) U_n^{(2l;\alpha\downarrow)}(-\mathbf{k}) U^{\dagger m}_{2l;\beta\downarrow}(-\mathbf{k}+\mathbf{q}) U_m^{(2l';\gamma\downarrow)}(-\mathbf{k}+\mathbf{q}) \frac{n_F(E_m(-\mathbf{k}+\mathbf{q}))-n_F(E_n(-\mathbf{k}))}{i\omega_n+E_m(-\mathbf{k}+\mathbf{q})-E_n(-\mathbf{k})}] \, .
\end{aligned}
\tag{12}
$$

The kinetic energy term for the superfluid stiffness can be obtained according to the method in sec. II, and we use it to calculate the renormalized factor g. The corresponding factors for different states are shown Fig. 1.