Supplementary Information

Local antiferromagnetic exchange and collaborative Fermi surface as key ingredients of high temperature superconductors

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We briefly discuss reciprocal pairing form factors provided by antiferromagnetic exchange interactions. Considering a magnetic exchange coupling between two electrons at two different sites, we have

$$J_{ij}\vec{S}_i\cdot\vec{S}_j=\frac{1}{4}\sum_{\sigma}[2J_{ij}c^{+}_{i\sigma}c^{+}_{j\sigma}c_{j\bar{\sigma}}c_{i\bar{\sigma}}+J_{ij}c^{+}_{i\sigma}c^{+}_{j\sigma}c_{j\sigma}c_{i\sigma}-J_{ij}c^{+}_{i\sigma}c^{+}_{j\bar{\sigma}}c_{j\bar{\sigma}}c_{i\sigma}] \tag{1}$$

where $\bar{\sigma}$ labels the opposite spin direction of σ. Given an antiferromagnetic exchange coupling $J_{ij}>0$, the decoupling of the first two terms in Eq. 1 in pairing channel leads to triplet pairing and costs energy. The last term in Eq. 1 gives singlet pair and saves energy. Defining $\Delta_{ij}=<c^{+}_{i\sigma}c^{+}_{j\bar{\sigma}}>$, we obtain that the energy saved from magnetic exchange coupling is given by

$$<J_{ij}\vec{S}_i\cdot\vec{S}_j>=-\frac{1}{2}J_{ij}|\Delta_{ij}|^2 \tag{2}$$

In a uniform superconducting state, Δ_{ij} should be a function of $\vec{r}_i-\vec{r}_j$. Therefore, we can define $\Delta_{\vec{k}}=\frac{1}{N}\sum_{<ij>}e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}\Delta_{ij}=<c^{+}_{\sigma}(\vec{k})c^{+}_{\bar{\sigma}}(-\vec{k})>$, where N is the total number of $<ij>$ links and $c^{+}_{\sigma}(\vec{k})$ is electron creation operators in momentum space.

First, we consider cases in a tetragonal lattice and define $\vec{x}$, $\vec{y}$ as the unit vectors of the lattice.

- s-wave pairing by NN AF in a tetragonal lattice:
  $\Delta_{ii\pm\vec{x}}=\Delta_{ii\pm\vec{y}}=\Delta_0$, $\Delta_{\vec{k}}=\frac{\Delta_0}{4}(e^{ik_x}+e^{-ik_x}+e^{ik_y}+e^{-ik_y})=\frac{\Delta_0}{2}(cosk_x+cosk_y)$.
- d-wave pairing by NN AF in a tetragonal lattice:
  $\Delta_{ii\pm\vec{x}}=-\Delta_{ii\pm\vec{y}}=\Delta_0$, $\Delta_{\vec{k}}=\frac{\Delta_0}{4}(e^{ik_x}+e^{-ik_x}-e^{ik_y}-e^{-ik_y})=\frac{\Delta_0}{2}(cosk_x-cosk_y)$.
- s-wave pairing by 2_{nd} NN AF in a tetragonal lattice:
  $\Delta_{ii\pm(\vec{x}\pm\vec{y})}=\Delta_0$, $\Delta_{\vec{k}}=\frac{\Delta_0}{4}(e^{ik_x+ik_y}+e^{-ik_x-ik_y}+e^{ik_x-ik_y}+e^{ik_y-ik_x})=\Delta_0cosk_xcosk_y$.
- d-wave pairing by 2_{nd} NN AF in a tetragonal lattice:
  $\Delta_{ii\pm(\vec{x}+\vec{y})}=-\Delta_{ii\pm(\vec{x}-\vec{y})}=\Delta_0$, $\Delta_{\vec{k}}=\frac{\Delta_0}{4}(e^{ik_x+ik_y}+e^{-ik_x-ik_y}-e^{ik_x-ik_y}-e^{ik_y-ik_x})=\Delta_0sink_xsink_y$.
- s-wave pairing by 3_{rd} NN AF in a tetragonal lattice:
  $\Delta_{ii\pm2\vec{x}}=\Delta_{ii\pm2\vec{y}}=\Delta_0$, $\Delta_{\vec{k}}=\frac{\Delta_0}{4}(e^{i2k_x}+e^{-i2k_x}+e^{i2k_y}+e^{-i2k_y})=\frac{\Delta_0}{2}(cos2k_x+cos2k_y)$.
- d-wave pairing by 3_{rd} NN AF in a tetragonal lattice:
  $\Delta_{ii\pm2\vec{x}}=-\Delta_{ii\pm2\vec{y}}=\Delta_0$, $\Delta_{\vec{k}}=\frac{\Delta_0}{4}(e^{i2k_x}+e^{-i2k_x}-e^{i2k_y}-e^{-i2k_y})=\frac{\Delta_0}{2}(cos2k_x-cos2k_y)$.

Second, we consider a standard triangle lattice with the two unit vectors $\vec{e}_1=(1,0),\vec{e}_2=(\frac{1}{2},\frac{\sqrt{3}}{2})$.

- s-wave pairing by NN AF in a triangle lattice:
  $\Delta_{ii\pm\vec{e}_1}=\Delta_{ii\pm\vec{e}_2}=\Delta_{ii\pm(\vec{e}_1-\vec{e}_2)}=\Delta_0$,
  $\Delta_{\vec{k}}=\frac{\Delta_0}{6}(e^{i\vec{k}\cdot\vec{e}_1}+e^{-i\vec{k}\cdot\vec{e}_1}+e^{i\vec{k}\cdot\vec{e}_2}+e^{-i\vec{k}\cdot\vec{e}_2}+e^{i\vec{k}\cdot(\vec{e}_1-\vec{e}_2)}+e^{-i\vec{k}\cdot(\vec{e}_1-\vec{e}_2)})=\frac{\Delta_0}{3}(cosk_x+2cos\frac{k_x}{2}cos\frac{\sqrt{3}}{2}k_y)$.
- $d\pm id$-wave pairing by NN AF in a triangle lattice:
  $\Delta_{ii\pm\vec{e}_1}=e^{\pm i\frac{2\pi}{3}}\Delta_{ii\pm\vec{e}_2}=e^{\pm i\frac{4\pi}{3}}\Delta_{ii\pm(\vec{e}_1-\vec{e}_2)}=\Delta_0$,
  $\Delta^{\pm}_{\vec{k}}=\frac{\Delta_0}{6}(e^{i\vec{k}\cdot\vec{e}_1}+e^{-i\vec{k}\cdot\vec{e}_1}+e^{\pm i\frac{2\pi}{3}}(e^{i\vec{k}\cdot\vec{e}_2}+e^{-i\vec{k}\cdot\vec{e}_2})+e^{\pm i\frac{4\pi}{3}}(e^{i\vec{k}\cdot(\vec{e}_1-\vec{e}_2)}+e^{-i\vec{k}\cdot(\vec{e}_1-\vec{e}_2)}))=\frac{\Delta_0}{3}(cosk_x-cos\frac{k_x}{2}cos\frac{\sqrt{3}}{2}k_y\pm i\sqrt{3}sin\frac{k_x}{2}sin\frac{\sqrt{3}}{2}k_y)$.

Finally, we consider a honeycomb lattice where the two unit vectors are given by $\vec{e}_1 = (\frac{\sqrt{3}}{2}, \frac{1}{2}), \vec{e}_2 = (\frac{\sqrt{3}}{2}, -\frac{1}{2})$. For convenience, we define $\vec{e}_0 = (-\frac{1}{\sqrt{3}}, 0)$.

- s-wave pairing by NN AF in a honeycomb lattice:
  $\Delta_{ii+\vec{e}_0} = \Delta_{ii+\vec{e}_0+\vec{e}_1} = \Delta_{ii+(\vec{e}_1+\vec{e}_2)} = \Delta_0$,
  $\Delta_{\vec{k}} = \frac{\Delta_0}{3}(e^{i\vec{k}\cdot\vec{e}_0} + e^{i\vec{k}\cdot(\vec{e}_0+\vec{e}_2)} + e^{i\vec{k}\cdot(\vec{e}_0+\vec{e}_2)}) = \frac{\Delta_0}{3} e^{-i\frac{1}{\sqrt{3}}k_x}(1 + 2cos(\frac{k_y}{2})e^{i\frac{\sqrt{3}}{2}k_x})$.
- $d{\pm}id$-wave pairing by NN AF in a honeycomb lattice:
  $\Delta_{ii\vec{e}_0} = e^{\pm i\frac{4\pi}{3}}\Delta_{ii\vec{e}_0+\vec{e}_1} = e^{\pm i\frac{2\pi}{3}}\Delta_{ii+(\vec{e}_0+\vec{e}_2)} = \Delta_0$,
  $\Delta_{\vec{k}} = \frac{\Delta_0}{3}(e^{i\vec{k}\cdot\vec{e}_0} + e^{\pm i\frac{2\pi}{3}}e^{i\vec{k}\cdot(\vec{e}_0+\vec{e}_2)} + e^{\pm i\frac{4\pi}{3}}e^{i\vec{k}\cdot(\vec{e}_0+\vec{e}_2)}) = \frac{\Delta_0}{3} e^{-i\frac{1}{\sqrt{3}}k_x}(1 + 2cos(\frac{k_y}{2} \pm \frac{2\pi}{3})e^{i\frac{\sqrt{3}}{2}k_x})$.
- s-wave pairing by 2_{nd} NN AF in a honeycomb lattice:
  $\Delta_{ii\pm\vec{e}_1} = \Delta_{ii\pm\vec{e}_2} = \Delta_{ii\pm(\vec{e}_1-\vec{e}_2)} = \Delta_0$,
  $\Delta_{\vec{k}} = \frac{\Delta_0}{6}(e^{i\vec{k}\cdot\vec{e}_1} + e^{-i\vec{k}\cdot\vec{e}_1} + e^{i\vec{k}\cdot\vec{e}_2} + e^{-i\vec{k}\cdot\vec{e}_2} + e^{i\vec{k}\cdot(\vec{e}_1-\vec{e}_2)} + e^{-i\vec{k}\cdot(\vec{e}_1-\vec{e}_2)}) = \frac{\Delta_0}{3}(cosk_y + 2cos\frac{k_y}{2}cos\frac{\sqrt{3}}{2}k_x)$.
- $d{\pm}id$-wave pairing by 2_{nd} NN honeycomb in a honeycomb lattice:
  $\Delta_{ii\pm\vec{e}_1} = e^{\pm i\frac{2\pi}{3}}\Delta_{ii\pm\vec{e}_2} = e^{\pm i\frac{4\pi}{3}}\Delta_{ii\pm(\vec{e}_1-\vec{e}_2)} = \Delta_0$,
  $\Delta^{\pm}_{\vec{k}} = \frac{\Delta_0}{6}(e^{i\vec{k}\cdot\vec{e}_1}+e^{-i\vec{k}\cdot\vec{e}_1}+e^{\pm i\frac{2\pi}{3}}(e^{i\vec{k}\cdot\vec{e}_2}+e^{-i\vec{k}\cdot\vec{e}_2})+e^{\pm i\frac{4\pi}{3}}(e^{i\vec{k}\cdot(\vec{e}_1-\vec{e}_2)}+e^{-i\vec{k}\cdot(\vec{e}_1-\vec{e}_2)})) = \frac{\Delta_0}{3}(cosk_y - cos\frac{k_x}{2}cos\frac{\sqrt{3}}{2}k_x \pm i\sqrt{3}sin\frac{k_y}{2}sin\frac{\sqrt{3}}{2}k_x)$.

We define the overlap between reciprocal form factors $\Delta_{\vec{k}}$ and Fermi surfaces as

$$W = \int\int dk_x dk_y |\Delta_{\vec{k}}|^2 \delta(\epsilon_{\vec{k}} - \mu) \tag{3}$$

To perform numerical calculations, we evaluate the above formular as follows

$$W = \frac{\int\int dk_x dk_y |\Delta_{\vec{k}}|^2 \Theta(\omega - |\epsilon_{\vec{k}} - \mu|)}{\int\int dk_x dk_y \Theta(\omega - |\epsilon_{\vec{k}} - \mu|)} \tag{4}$$

where ω is a small positive value that is much less than the band width and $\Theta(x)$ is the unit step function defined as $\Theta(x) = 1(0)$ if $x > 0 (x \leq 0)$. W has very week dependence on ω. For a multi-band system with N bands, we evaluate W_α for each band and define the average weight as $W = \frac{\sum_\alpha W_\alpha}{N}$. This average weight is a good quantity to evaluate approximately the overlap strength in iron-based superconductors since the gap functions of all the bands are fitted to a single pairing form function as discussed in this paper.

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