Superconductivity and Spin Fluctuations in Iron Pnictides: FLEX Study
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Motivation
Understanding of mechanism of superconductivity in iron pnictides
\begin{itemize}
  \item 5-band Hubbard model
  \item Non-local correlations on bct-bct ladder level - fluctuation exchange (FLEX)
\end{itemize}

Questions we address:
\begin{itemize}
  \item Leading 2-particle instability (superconductivity vs magnetism)
  \item Doping and temperature dependent trends
  \item Normal state spin dynamics
\end{itemize}

5-band model for LaOFeAs

Starting from LDA bandstructure of undoped LaOFeAs for experimental lattice parameters we construct a 5-band model in unfolded Brillouin zone. We use on-site Coulomb interaction in Slater-Kanemori parametrization. We want $U$ and $J$ as two parameters.

Undoped system

The static spin susceptibility for two values of the on-site repulsion at $T=35$ K. The peaks at $(\pi,0)$ are precursors of the stripe order.

FLEX

Self-consistent weak-coupling perturbative method. Consists in replacing the $sp$- and $p$-orbitadue vertices with their bare value and self-consistent solution of Bethe-Salpeter, Schwinger-Dyson and Dyson equations.
\begin{itemize}
  \item 1-particle self-energy contains all bubble and ladder sums.
  \item Non-local reducible vertices are generated.
  \item Pairing vertices are generated.
\end{itemize}

\textbf{Poor man's double counting} - allows only minor modification of the non-interacting Fermi surface:
\begin{align*}
\Delta_{c}(k,i\omega_{n}) &= \Delta_{c}(k,i\omega_{n}) - Re \, \Sigma_{c}(k,i\omega_{n})
\end{align*}

Leading 2-particle instabilities:
\begin{enumerate}
  \item Spin ordering
    \begin{align*}
    \tilde{X}(q) &= \tilde{X}(q) + \tilde{X}(q) \tilde{X}(q) \\
    \tilde{X}(q) &= \sum_{\alpha} \tilde{X}_{\alpha}(q)
    \end{align*}
    (Bethe-Salpeter eq.)
    Magnetic instability: $\xi_{c}=100$
    Pairing instability: $\lambda=1$
  \item Superconductivity
    \begin{align*}
    \Delta_{s}(k) &= \mathcal{N} \int_{\omega_{n}} \frac{d\omega_{n}}{\pi} \frac{1}{2} \sum_{\alpha} \tilde{X}_{\alpha}(k+i\omega_{n}) \tilde{X}_{\alpha}(k+i\omega_{n}) \Delta_{s}(k+i\omega_{n}) \\
    \end{align*}
\end{enumerate}

Effect of doping

Evolution of the Fermi surface as a function of the electron filling. Electron sheets are marked in green, hole sheets in red, orange and yellow.

The static spin susceptibility for hole and electron doping.

Doping dependence of the Eliashberg eigenvalue $\lambda$ and the spin susceptibility $\chi_{\alpha}(q,0)$ at 35 K.

Upon electron doping above 6.15 the $\Gamma$ sheet disappears and the low-energy spin fluctuations become dominated by scattering between different $M$ sheets.

Summary

\begin{itemize}
  \item FLEX is a weak coupling approach and thus provides a description qualitatively similar to non-selfconsistent RPA, i.e. description in terms of Fermi surface geometries.
  \item It takes into account variation of orbital character over the Fermi surface and $T$, $k$- and orbital-dependent renormalization of quasiparticles.
  \item Both magnetic ordering and superconductivity are driven by Fermi surface nesting. A perfect nesting picks a single $q$ and thus favors magnetic ordering, the superconducting pairing can make use of a whole $(q,\omega)$-range of strong spin fluctuation modes and thus is favored by near nesting.
  \item The preferred pairing mode in the hole-doped region is $\pi$ with a small amplitude variation over FS sheets. In the electron-doped region the $\pm$ exhibits a large amplitude variation and eventually is replaced with $d_{x^2-y^2}$. The spin-dipole fluctuations account for 60-70\% of the pairing while the rest comes from higher spin multipoles.
\end{itemize}