Interplay of charge density wave, pairing density wave and superconductivity in high Tc cuprate superconductors

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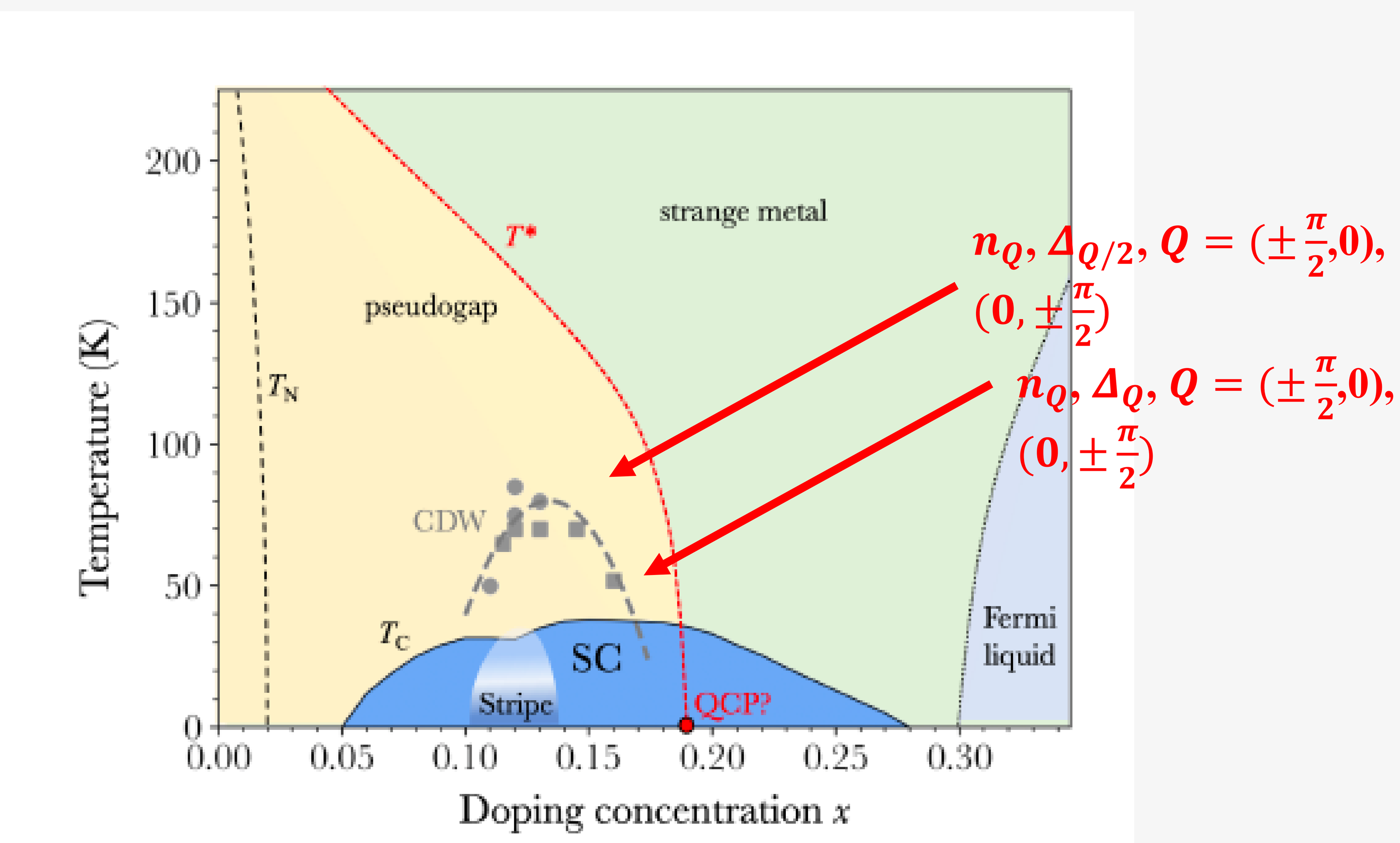
Abstract

In this work, We study the interplay among charge density wave (CDW), pair density wave (PDW), and d-wave superconducting (SC) orders in high-temperature cuprate superconductors. Using the renormalized mean-field theory based on the t-J model formulated in real space, we derive self-consistent equations incorporating for CDW, PDW and d-wave SC order parameters with different doping. We focus on wavevectors Q=(Qx,Qy) and their multiples (nQx,mQy) with Qx=Qy=pi/4 and m, n=0,+/-1, +/-2…+/-7 . The results show that density waves are dominated by wavevectors being pi/4 and its multiples in the underdoped regime, and they are dominated by wavevectors being pi/4 and its multiples around the optimum doping regime. Furthermore, density waves continue to the overly doped regime and vanish at doping being around 0.19, displaying the quantum critical point at doping level 0.19.

Motivation



Our approach: renormalized mean-field theory (RMFT)

We introduce the t − J model on a square lattice of Cu

$$H = -\sum_{\langle i,j\rangle,\sigma} P_G t_{ij}\left(c_{i\sigma}^\dagger c_{j\sigma} + H.C.\right)P_G + \sum_{\langle i,j\rangle} J\, S_i \cdot S_j$$

where $P_G = \prod_i (1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$ is the Gutzwiller projection factors, hopping term t_{ij} is equal to t and t' are nearest and next nearest neighbor sites. $t' = -0.3t$ and $t' = 0.3t$ are used in this study.

Compare with original Hartree–Fock type wavefunction (unprojected wave function $|\psi_0\rangle$), the projected wave-function and the expected value of the operator

$$|\psi\rangle = P_G|\psi_0\rangle$$

$$\langle\hat{O}\rangle \equiv \frac{\langle\psi|\hat{O}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\langle\psi_0|P_G\hat{O}\,P_G|\psi_0\rangle}{\langle\psi_0|P_G P_G|\psi_0\rangle}$$

This projection operator eliminates all double-occupancy components from each lattice site.

Since the projection operator is difficult to treat analytically, the Gutzwiller approximation is developed to renormalize the Hamiltonian and expectation value. The projection operator P_G is replaced by the Gutzwiller renormalization factors

$$\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle = g_t\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle_0, \qquad \langle S_i \cdot S_j\rangle = g_s\langle S_i \cdot S_j\rangle_0$$

g_t and g_s are the renormalization factors of the corresponding expectation values, and corrections are

$$t_{\rm eff} = g_t t, \qquad J_{\rm eff} = g_s J$$

Following the idea of Gutzwiller and work of Himeda and Ogata (anti-ferromagnetism (AF) order), The renormalized Hamiltonian and renormalization factors become

$$H = -\sum_{i,j,\sigma} g_{ij}^t t_{ij}\left(c_{i\sigma}^\dagger c_{j\sigma} + H.C.\right) + \sum_{\langle i,j\rangle} J\left[g_{ij}^{s,z} S_i^z S_j^z + \frac{g_{ij}^{s,xy}\left(S_i^+ S_j^- + S_i^- S_j^+\right)}{2}\right]$$

g_{ij}^t, $g_{ij}^{s,z}$, $g_{ij}^{s,xy}$ are the Gutzwiller factors considering the coexistence of anti-ferromagnetism (AF) and d-wave superconductivity, which are dependent on the values of local AF moment m_i^v, pair field $\Delta_{ij\sigma}^v$, bond order $\chi_{ij\sigma}^v$, and hole density δ_i

$$m_i^v = \langle\Psi_0|S_i^z|\Psi_0\rangle$$

$$\Delta_{ij\sigma}^v = \sigma\langle\Psi_0|c_{i\sigma}c_{j\sigma}|\Psi_0\rangle$$

$$\chi_{ij\sigma}^v = \langle\Psi_0|c_{i\sigma}^\dagger c_{j\sigma}|\Psi_0\rangle$$

$$\delta_i = 1 - \langle\Psi_0|n_i|\Psi_0\rangle$$

$$g_{i,j,\sigma}^t = g_{i,\sigma}^t g_{j,\sigma}^t$$

$$g_{i,\sigma}^t = \sqrt{\frac{2\delta_i(1-\delta_i)}{1-\delta_i^2+4m_i^2}\left(\frac{1+\delta_i+\sigma\,2m_i}{1+\delta_i-\sigma\,2m_i}\right)}$$

$$g_{i,j}^{s,xy} = g_i^{s,xy} g_j^{s,xy}, \qquad g_i^{s,xy} = \frac{2(1-\delta_i)}{1-\delta_i^2+4m_i^2}$$

$$g_{i,j}^z = g_{i,j}^{s,xy}\left(\frac{2\left(\Delta_{i,j}^2+\chi_{i,j}^2\right) - 4m_i m_j X_{i,j}^2}{2\left(\Delta_{i,j}^2+\chi_{i,j}^2\right) - 4m_i m_j}\right)$$

$$X_{i,j} = 1 + 12(1-\delta_i)(1-\delta_j)\left(\Delta_{i,j}^2+\chi_{i,j}^2\right)\Big/\sqrt{\left(1-\delta_i^2+4m_i^2\right)\left(1-\delta_j^2+4m_j^2\right)}$$

Reference

1. Gutzwiller, Phys. Rev. Lett. 10, 159–162 (1963).
2. Ogata, M. & Himeda, J. Phys. Soc. Japan 72, 374–391 (2003).

Iterative method

We solve self-consistent the real space mean-field Hamiltonian for all the parameters above-mentioned

$$H_{MF} = \left(c_{i\uparrow}^\dagger, c_{i\downarrow}\right)\begin{pmatrix} H_{ij\uparrow} & D_{ij} \\ D_{ji}^* & -H_{ji\downarrow}\end{pmatrix}\begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}^\dagger\end{pmatrix}$$

Performing several iterations (200~400 times), the convergence of difference between successive iterations can achieve for 10^{-5}~10^{-6}. The order parameters in system can obtain by following eqations

$$n_{i\uparrow} = \langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle_0 = \sum_{n-}|u_i^n|^2, \qquad n_{i\downarrow} = \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle_0 = \sum_{n+}|v_i^n|^2$$

$$\Delta_{ij\uparrow}^v = \langle c_{i\uparrow}c_{j\downarrow}\rangle_0 = \sum_{n+} u_i^n v_j^{n*}, \qquad \Delta_{ij\downarrow}^v = -\langle c_{i\downarrow}c_{j\uparrow}\rangle_0 = \sum_{n+} u_j^n v_i^{n*}$$

$$\chi_{ij\uparrow}^v = \langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle_0 = \sum_{n-} u_j^n u_i^{n*}, \qquad \chi_{ij\downarrow}^v = \langle c_{i\downarrow}^\dagger c_{j\downarrow}\rangle_0 = \sum_{n+} v_i^n v_j^{n*}$$

To transform real space to k space, wea pply the Fourier Transform $\Delta_{ij\sigma}$ to obtain Δ_k, n_i to obtain n_k. The order parameter of charge density wave (CDW) and pair density wave (PDW) is defined by

CDW : $n_q = \sum_{k,\sigma}\langle c_{k+q,\sigma}^\dagger c_{k,\sigma}\rangle$, PDW : $\Delta_{q(k)} = \langle c_{k+q,\uparrow}c_{-k,\downarrow}\rangle$ $\quad q = 0, \pm\frac{\pi}{4}, \pm\frac{\pi}{2}, \pm\frac{3\pi}{4}$

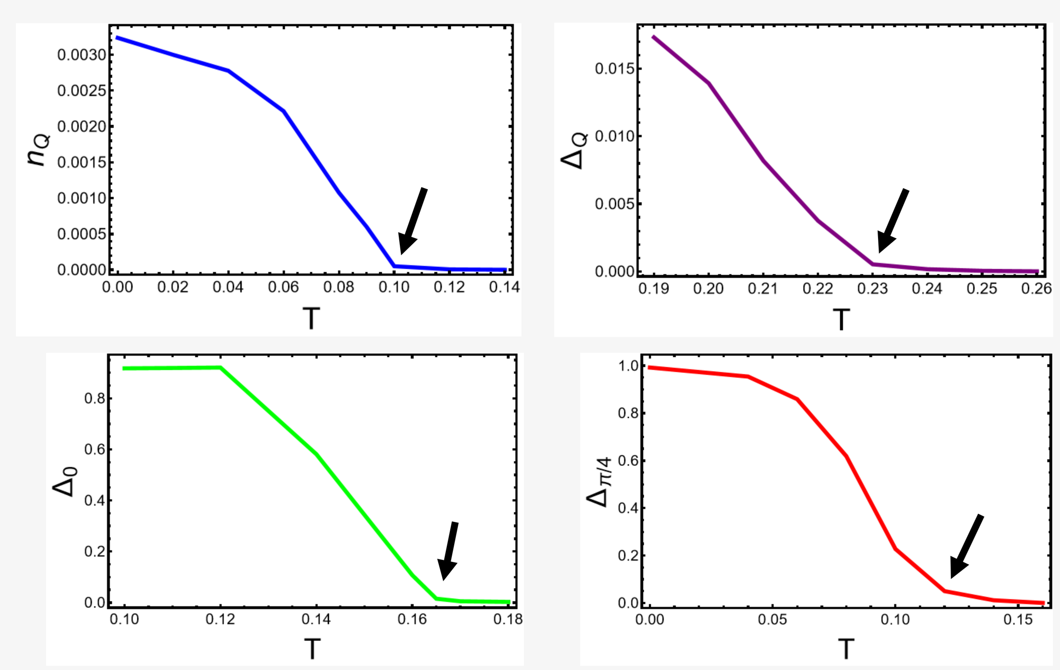
Here we choose Q=π/2

$n_{Q=\pi/2} = \sum_{k,\sigma}\langle c_{k+Q,\sigma}^\dagger c_{k,\sigma}\rangle$, $\quad \Delta_{Q(k)} = \sum_{k,\sigma}\langle c_{k+\frac{Q}{2},\uparrow} c_{-k+\frac{Q}{2},\downarrow}\rangle$

First, we calculate the real-space fields $n(r)$, $\Delta(r)$ on 8×8 lattice. Then perform Fourier transform to k space and obtain their Fourier components $n(q)$, $\Delta(q)$. For 8 × 8 lattice with periodic boundary conditions, the allowed wavevectors q=0, ±π/4, ±π/2, ±3π/4 from which we read off n_q, Δ_q.

$$n_q = \left(\frac{1}{N}\right)\sum_i n_i e^{-iq\cdot r_i}, \qquad \Delta_q = \left(\frac{1}{N}\right)\sum_i \Delta_i e^{-iq\cdot r_i}$$

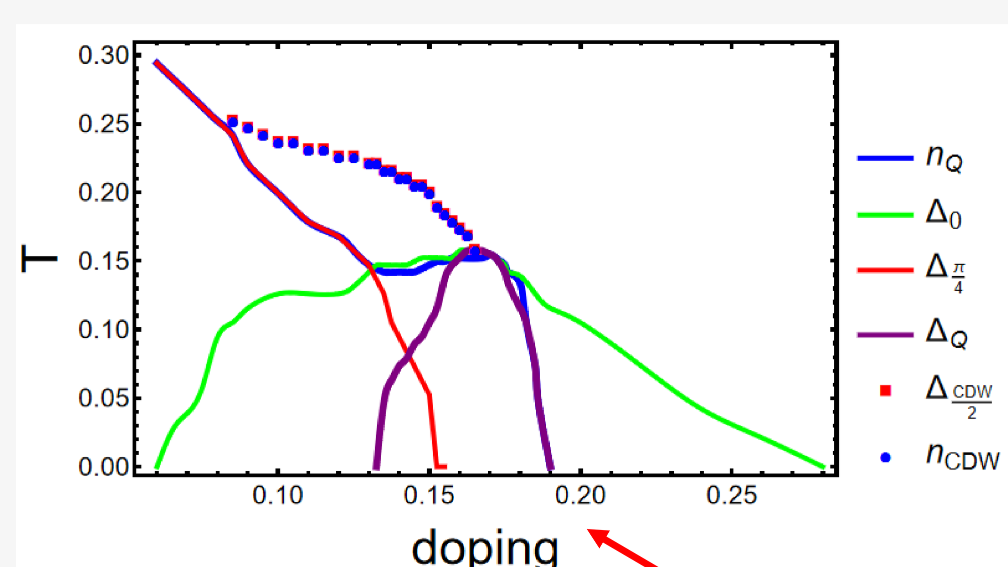
After Fourier transform, we obtain n_q, Δ_q. We then try a 12 × 12 lattice simulation, and the results are consistent with those for the 8 × 8 lattice



$n_{3\pi/4}$	$\Delta_{3\pi/4}$
$n_{Q=\pi/2}$ (CDW)	$\Delta_{Q=\pi/2}$(PDW)
$n_{\pi/4}$	$\Delta_{\pi/4}$
n_0	Δ_0(S.C)
$n_{-\pi/4}$	$\Delta_{-\pi/4}$
$n_{-Q=-\pi/2}$(CDW)	$\Delta_{-Q=-\pi/2}$(PDW)
$n_{-4\pi/4}$	$\Delta_{-4\pi/4}$
$n_{-\pi}$	$\Delta_{-\pi}$

Phase diagram

Parameters : t=1, t'=-0.3, J=0.3



Quantum critical point (QCP)

n_Q, Δ_Q, Δ_0 coexistence region : doping: 0.13~0.19 $\rightarrow \Delta_0\Delta_{-Q}n_Q$

$n_Q, \Delta_{\pi/4}$ coexistence region : doping: < 0.13 $\rightarrow n_Q\Delta_{Q/2}\Delta_{-Q/2}$

CDW regime : Blue and red dot $\rightarrow n_Q\Delta_{Q/2}\Delta_{-Q/2}$

Conclusion

1. We studied the interplay between CDW (n_Q), PDW (Δ_Q), and uniform d-wave superconductivity (Δ_0) within RMFT for the t–J model.
2. By extracting Fourier components from an 8×8 lattice, we resolved density-wave and pairing modulations at discrete wavevectors Q=mπ/4.
3. In the underdoped regime, the dominant density-wave components are mainly at Q=π/4 (and its multiples), while they shift toward Q=π/2 components near optimal doping.
4. The coexistence region of CDW, PDW and SC appears in an intermediate doping range
5. Both CDW and PDW amplitudes are suppressed upon overdoping, vanishing near δ≈0.19. this is the characteristic of quantum critical point (QCP)
6. We see some CDW order at high temperature, can be compered with experimental data.