Cooper approach to pair formation in a tight-binding model of La-based cuprate superconductors

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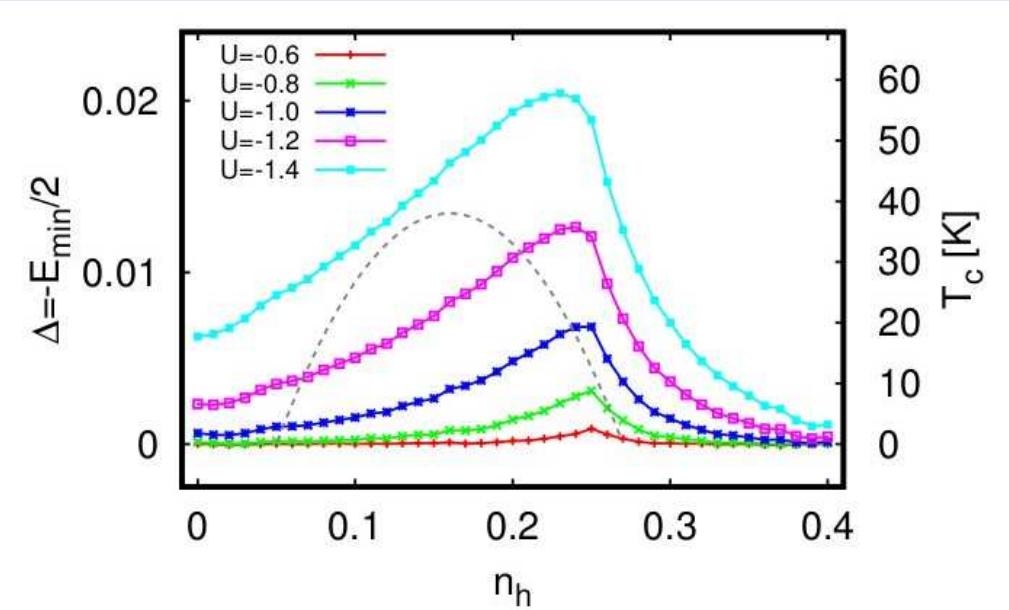

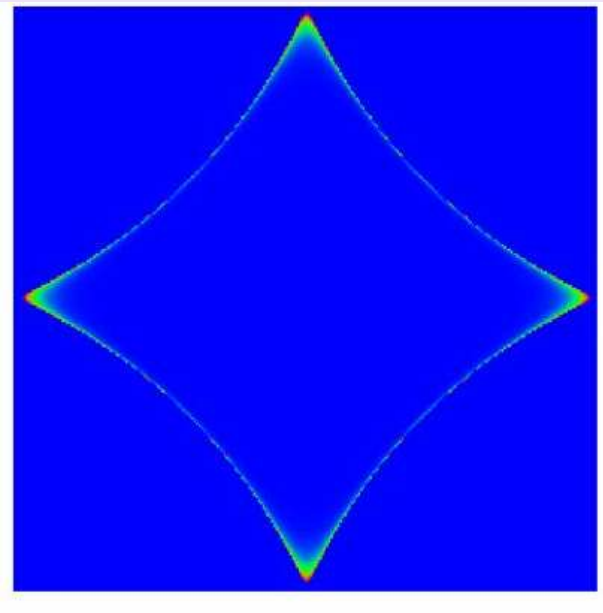

Cooper 1956: two interacting particles above a frozen Fermi sea; LSCO: static/mobile pairs at Hubbard attraction, d-wave type attraction, Coulomb repulsion; arXiv:2209.09057, [PRR **2**, 023354 (2020); EPJB **94**, 29 (2021)]

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Tight-binding model for La-based cuprate superconductors

ORIGINAL PAPER

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A 3D Tight-Binding Model for La-Based Cuprate Superconductors

*Raphaël Photopoulos and Raymond Frésard**

Ann.Phys.(Berlin) **2019**, 1900177 (2019) + Markiewicz,Bansil et al PRB(2005)

$t = 1 \rightarrow 0.43eV$; $t' = -0.136$, $t'' = 0.068$, $t''' = 0.061$, $t^{(4)} = -0.017$; $\hbar = 1$

$La_{2-x}Sr_xCuO_4 \rightarrow LSCO$ hole dopping

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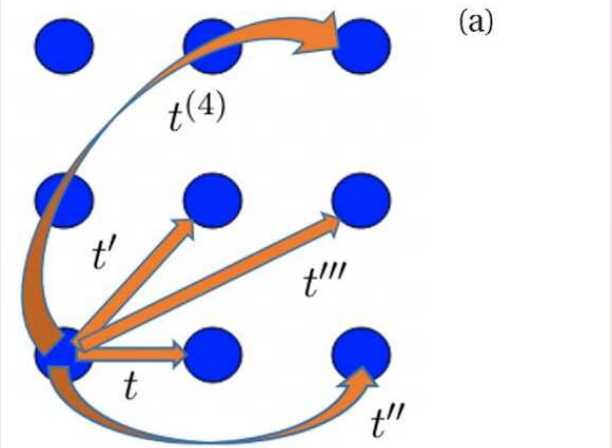

$$
\begin{aligned}
E_{1p}(p_x, p_y) = &-2\left[\cos(p_x) + \cos(p_y)\right] \\
&- 4t' \cos(p_x)\cos(p_y) \\
&- 2t''\left[\cos(2p_x) + \cos(2p_y)\right] \\
&- 4t'''\left[\cos(2p_x)\cos(p_y) + \cos(2p_y)\cos(p_x)\right] \\
&- 4t^{(4)} \cos(2p_x)\cos(2p_y)
\end{aligned}
$$

Hamiltonian of two interacting particles (TIP)

The quantum Hamiltonian of the model with two interacting particles (TIP) has the form:

$$H = H_{1p}^{(1)} \otimes \mathbf{1}^{(2)} + \mathbf{1}^{(1)} \otimes H_{1p}^{(2)} + \sum_{\mathbf{r}_1, \mathbf{r}_2} \bar{U}(\mathbf{r}_2 - \mathbf{r}_1) |\mathbf{r}_1, \mathbf{r}_2\rangle\langle \mathbf{r}_1, \mathbf{r}_2| \tag{4}$$

where $H_{1p}^{(j)}$ is the one-particle Hamiltonian (1) of particle $j = 1, 2$ with positional coordinate $\mathbf{r}_j = (x_j, y_j)$ and $\mathbf{1}^{(j)}$ is the unit operator of particle j. The last term in (4) represents a (regularized) Coulomb type long-range interaction $\bar{U}(\mathbf{r}_2 - \mathbf{r}_1) = U/[1 + r(\mathbf{r}_2 - \mathbf{r}_1)]$ with amplitude U and the effective distance $r(\mathbf{r}_2 - \mathbf{r}_1) = \sqrt{\Delta\bar{x}^2 + \Delta\bar{y}^2}$

Interactions:

* - attractive Hubbard $U(r_1, r_2) = U\delta_{r_1, r_2}$;

* - attractive d-wave in momentum space $U(p_1, p_2) = U g_{k_1} g_{k_2}$ ($g_{k_{1,2}} = (\cos k_{1,2x} - \cos k_{1,2y})/2$ inside sector of fixed $p_+ = const$; $p = k$);

* - Coulomb repulsion

Total momentum $p_+ = p_1 + p_2$ is conserved;

static ($p_+ = 0$) and mobile ($p_+ \neq 0$) pairs if compact in coordinate space

Hamiltonian of two interacting particles (TIP)

Without interaction ($U = 0$) the energy eigenvalues of the two electron Hamiltonian (4) with given momenta $\mathbf{p}_1$ and $\mathbf{p}_2$ are:

$$E_c(\mathbf{p}_1, \mathbf{p}_2) = E_{1p}(\mathbf{p}_1) + E_{1p}(\mathbf{p}_2) = -4 \sum_{\mathbf{a} \in \mathcal{A}} t_{\mathbf{a}} \cos(\mathbf{p}_+ \cdot \mathbf{a}/2) \cos(\Delta\mathbf{p} \cdot \mathbf{a}) \quad (5)$$

where $\mathbf{p}_+ = \mathbf{p}_1 + \mathbf{p}_2$ is the total momentum and $\Delta\mathbf{p} = (\mathbf{p}_2 - \mathbf{p}_1)/2$ is the momentum associated to the relative coordinate $\Delta\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$. For the NN model Eq. (5) becomes $E_c(\mathbf{p}_1, \mathbf{p}_2) = -4 \sum_{\alpha=x,y} \cos(p_{+\alpha}/2) \cos(\Delta p_\alpha)$.

Effective narrow or flat band when $\cos(p_{+x,+y}/2) \approx 0 \rightarrow$ even repulsive particles cannot become separated due to energy conservation and form a pair

Frahm, DS PRR **2**, 023354 (2020); EPJB **94**, 29 (2021)

Cooper approach: frozen Fermi sea (1956)

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Bound Electron Pairs in a Degenerate Fermi Gas*

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(Received September 21, 1956)

IT has been proposed that a metal would display superconducting properties at low temperatures if the one-electron energy spectrum had a volume-independent energy gap of order $\Delta \simeq kT_c$, between the ground state and the first excited state.[1,2] We should like to point out how, primarily as a result of the exclusion principle, such a situation could arise.

Consider a pair of electrons which interact above a quiescent Fermi sphere with an interaction of the kind

tron two. (One can use antisymmetric functions and obtain essentially the same results, but alternatively we can choose the electrons of opposite spin.) Defining relative and center-of-mass coordinates, $\mathbf{R}=\frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$, $\mathbf{r}=(\mathbf{r}_2-\mathbf{r}_1)$, $\mathbf{K}=(\mathbf{k}_1+\mathbf{k}_2)$ and $\mathbf{k}=\frac{1}{2}(\mathbf{k}_2-\mathbf{k}_1)$, and letting $\mathcal{E}_K+\epsilon_k=(\hbar^2/m)(\frac{1}{4}K^2+k^2)$, the Schrödinger equation can be written

$$(\mathcal{E}_K+\epsilon_k-E)a_{\mathbf{k}}+\sum_{\mathbf{k}'} a_{\mathbf{k}'}(\mathbf{k}|H_1|\mathbf{k}') \times\delta(\mathbf{K}-\mathbf{K}')/\delta(0)=0 \quad (1)$$

where

$$\Psi(\mathbf{R},\mathbf{r})=(1/\sqrt{V})e^{i\mathbf{K}\cdot\mathbf{R}}\chi(\mathbf{r},K), \qquad \chi(\mathbf{r},K)=\sum_{\mathbf{k}} (a_{\mathbf{k}}/\sqrt{V})e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2)$$

and

$$(\mathbf{k}|H_1|\mathbf{k}')=\left(\frac{1}{V}\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}H_1 e^{i\mathbf{k}'\cdot\mathbf{r}}\right)_{0 \text{ phonons}}.$$

We have assumed translational invariance in the metal. The summation over $\mathbf{k}'$ is limited by the exclusion principle to values of k_1 and k_2 larger than q_0, and by the delta function, which guarantees the conservation of the total momentum of the pair in a single scattering. The K dependence enters through the latter restriction.

Cooper case: quadratic spectrum $E = ({p_1}^2 + {p_2}^2)/2 = ({p_+}^2/4 + {p_-}^2)$
for LSCO $E(p_+, p_-)$ is a complex function of p_+, p_-
static pairs $p_+ = 0$, mobile pairs $p_+ \neq 0$

Fermi surface of LSCO

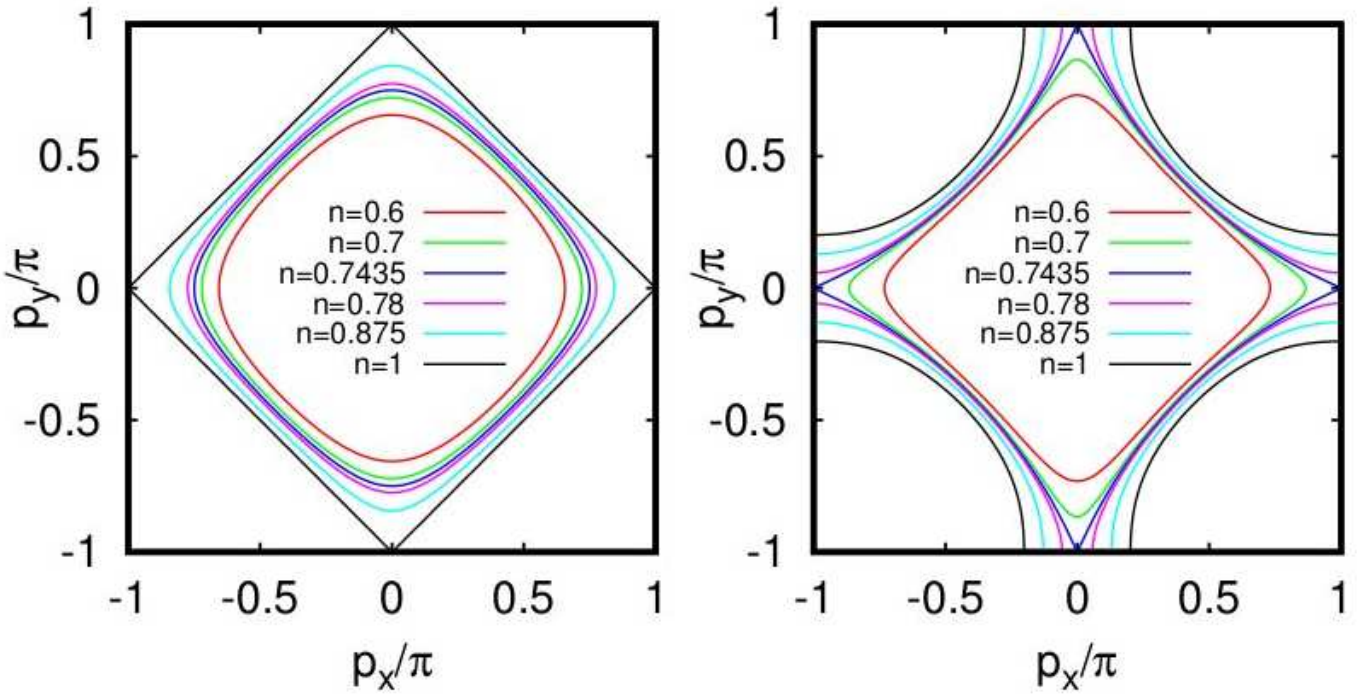


Fig. Fermi surface for different filling factors n for the NN model (left panel) and the HTC model (right panel). The value $n = 0.7435$ is close to the separatrix value $n = 0.743465958$ for the HTC model and $n = 1$ is the separatrix value for the NN model.

Van Hove singularity (separatrix) of density of states at filling factor $n = 0.74346...$ (left nearest-neighbor (NN) model, right HTC model of LSCO)

Frozen Fermi sea of LSCO

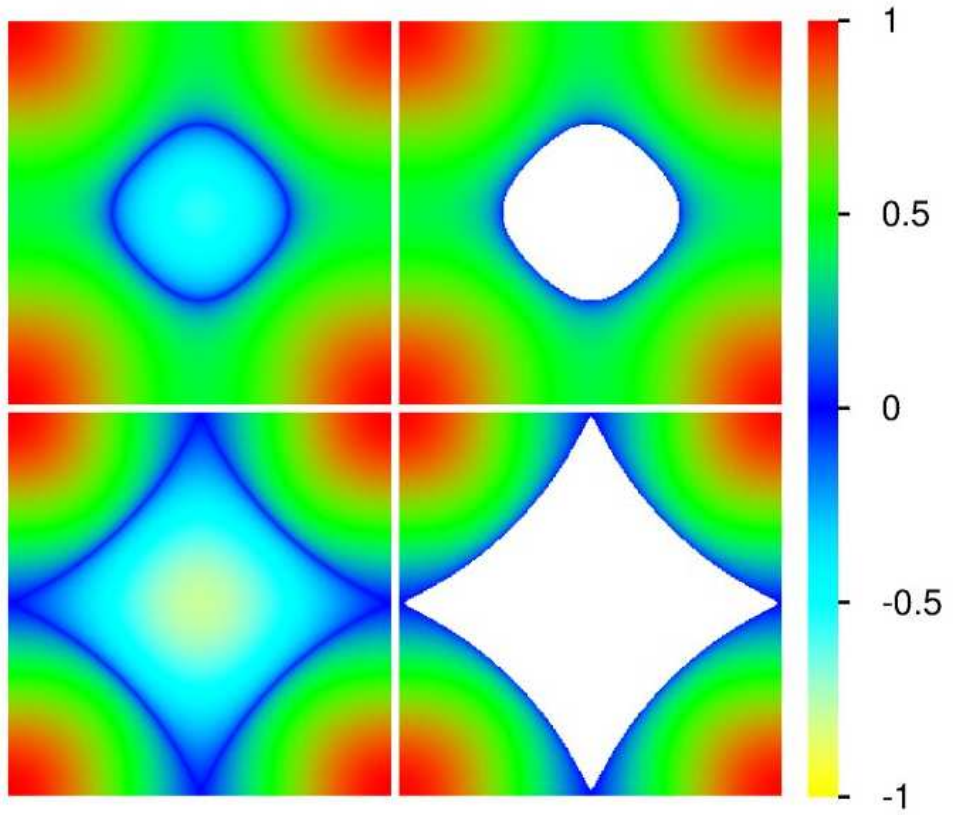
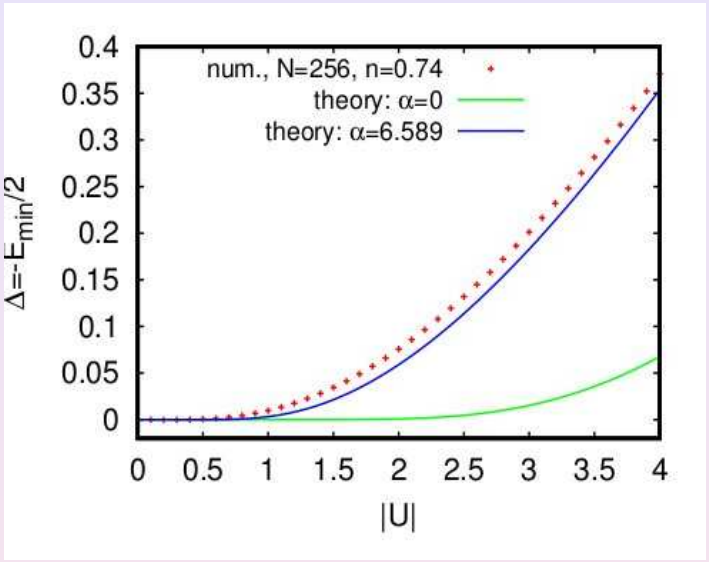
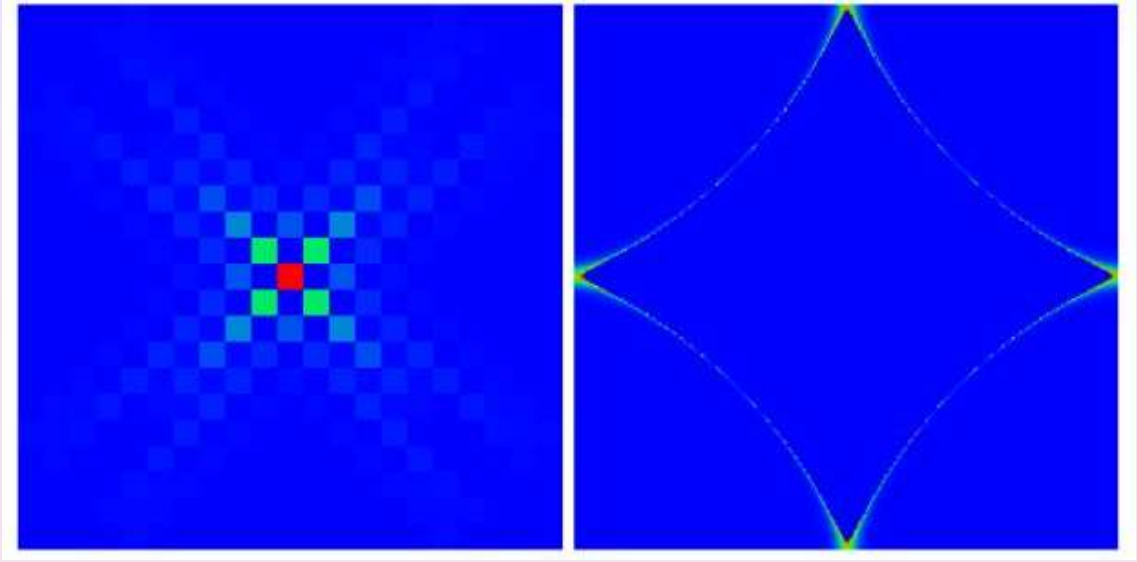


Fig. Landscape of energy of pair E_c for different relative momenta of particles $\Delta\vec{p}$. Left panels show color plots of $E_c(\vec{p}_+/2 - \Delta\vec{p}, \vec{p}_+/2 + \Delta\vec{p}) - 2E_F$ for the HTC model in the Δp_x-Δp_y plane for $-\pi \leq \Delta p_{x,y} < \pi$ in the sector $\vec{p}_+ = 0$. The Fermi energy E_F corresponds to the filling factor $n = 0.3$ ($n = 0.74$) for top (bottom) panels. The

Static pairs at $p_+ = 0$; filling factor $n = 0.3; 0.74$ (top; bottom)

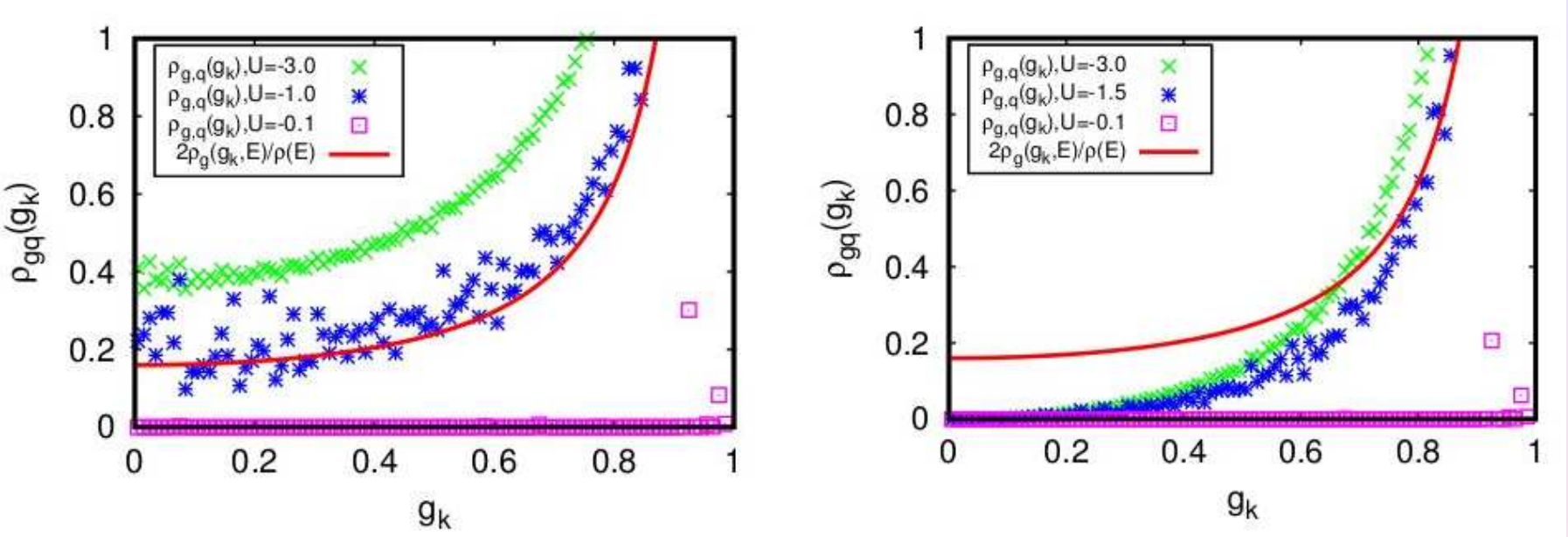
Gap dependence on U





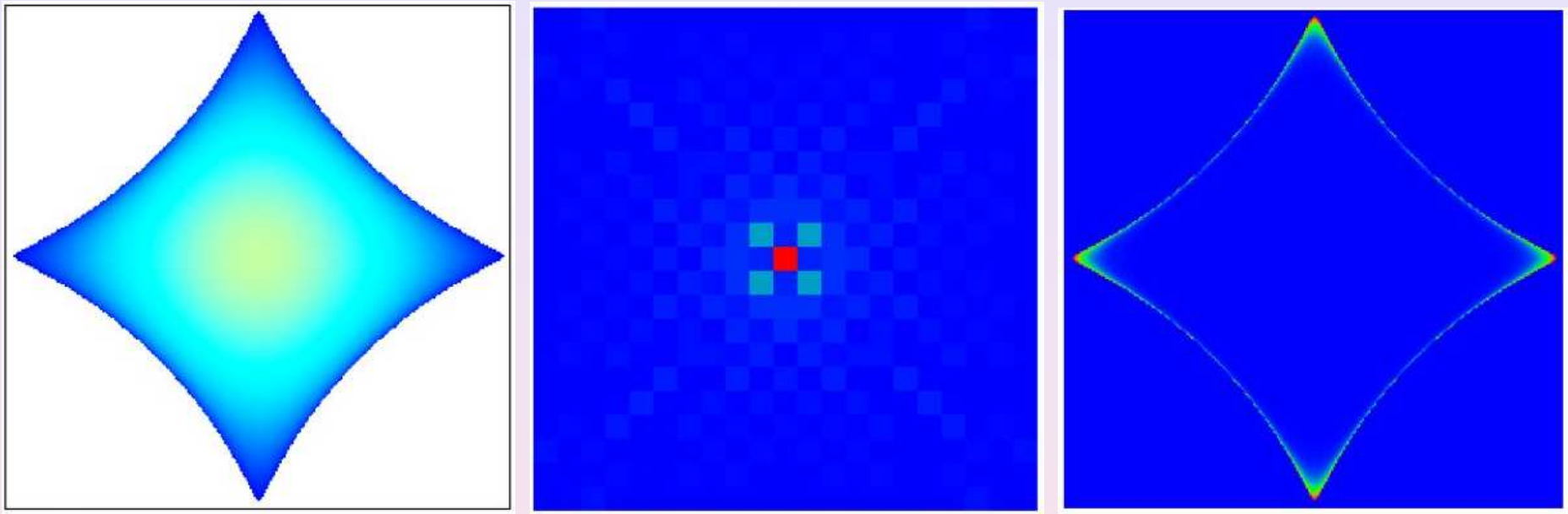
Static electron pairs at $p_+ = 0$, $n = 0.74$ Hubbard case, $\Delta(U)$ (left);
ground state $U = -1.$, $-10 \leq \Delta x, \Delta y \leq 10$ (center);
ground state in momentum $-\pi \leq \Delta p_{x,y} < \pi$ (right)
efficient numerical method for ground state
with $N \times N = 1024 \times 1024 > 10^6$ sites

Local density of states on Fermi surface



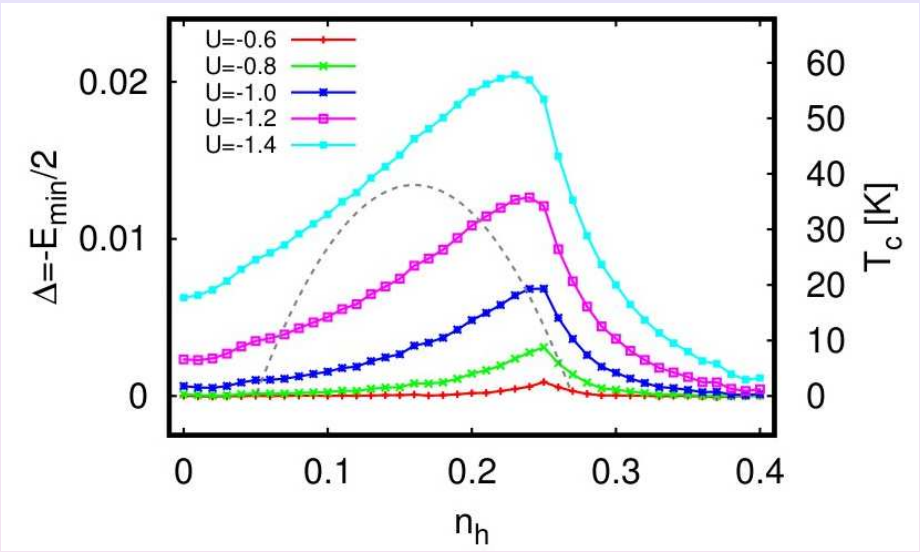
Ground state of static electron pairs at $p_+ = 0$, $n = 0.74$
Hubbard (left), d-wave interaction $g_k = (\cos k_x - \cos k_y)/2$ (right)
local density of states on Fermi surface: $\rho_g(g_k, E_F) = \rho_\varphi(\varphi, E_F)/(dg_k/d\varphi)$
red curve is from classical ergodic area of phase space

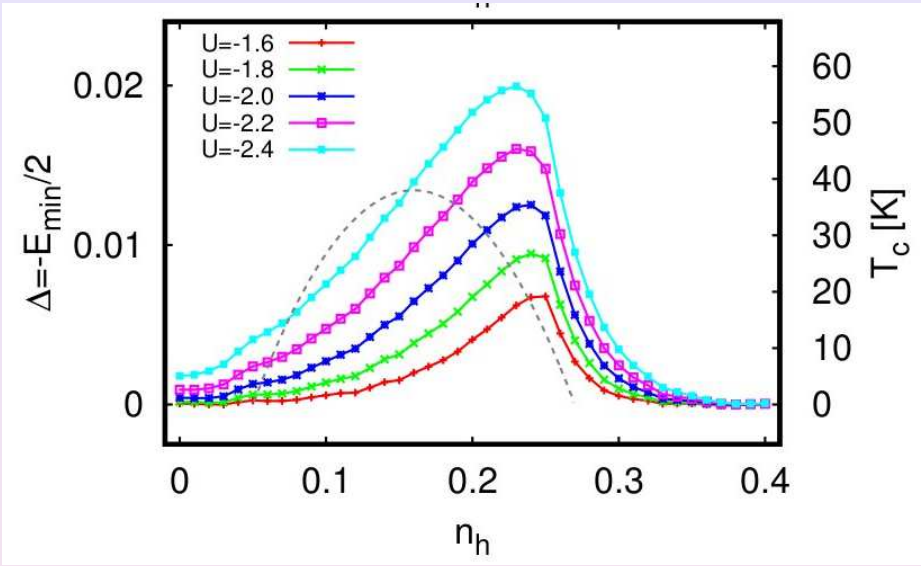
Ground state of holes (separatrix case)



Ground state of static hole pairs at $p_+ = 0$, $n_h = 1 - n = 0.26$, $N = 256$, $U = -1.5$ Hubbard interaction:
accessible Fermi area in momentum (left); ground state in coordinate space (zoom at (-10,10) - center); ground state in momentum $(-\pi, \pi)$

Gap dependence on hole dopping in LSCO





Static hole pairs at $p_+ = 0$, hole dopping $n_h = 1 - n$

Gap $\Delta = 1.764 k_B T_c$ or critical temperature T_c vs hole dopping n_h

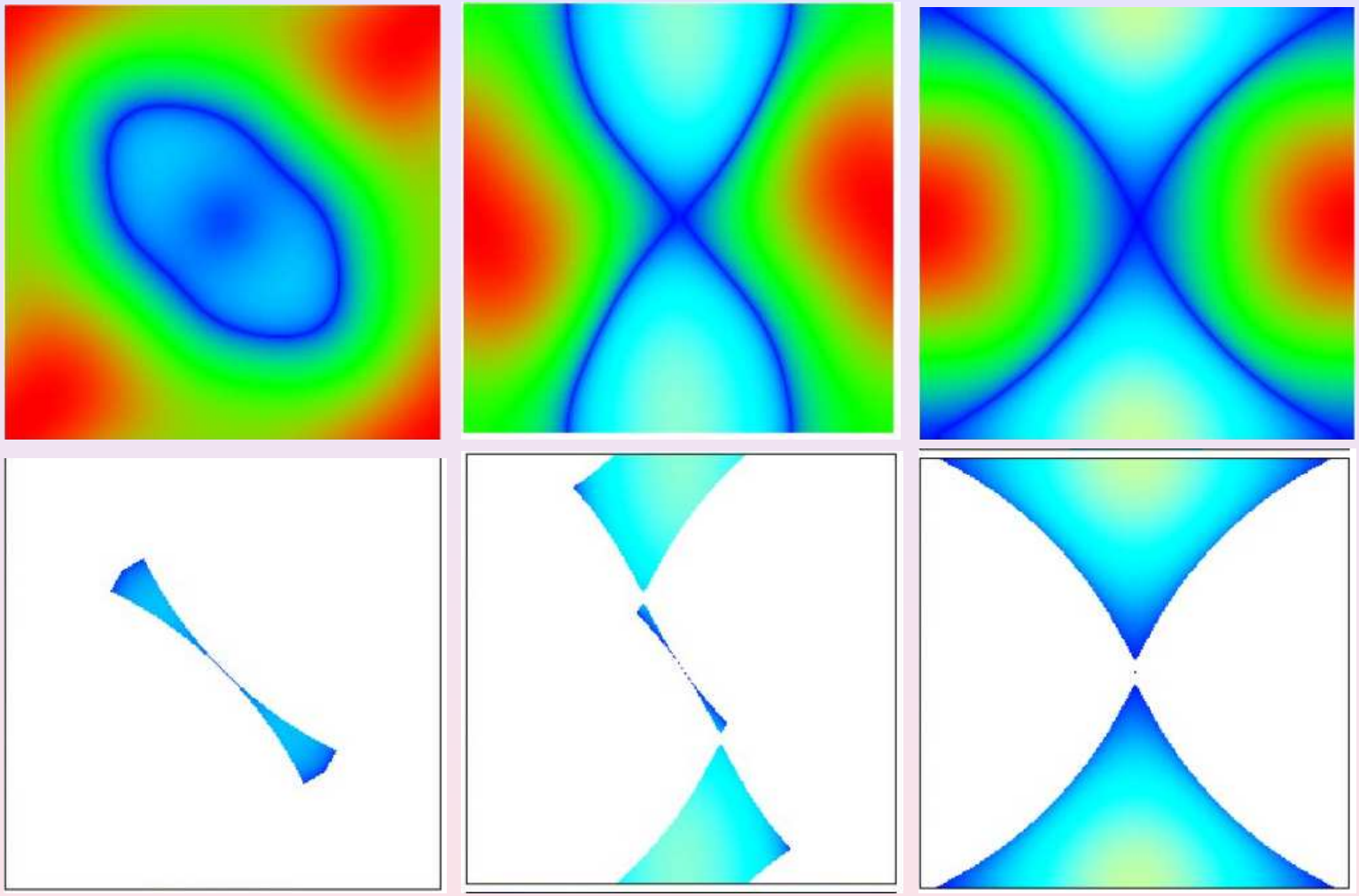
Hubbard (left), d-wave interaction $g_k = (\cos k_x - \cos k_y)/2$ (right)

Dashed black curve: LSCO experimental results with optimal dopping $n_h = 0.16$, max $T_c = 38K$ Markiewicz, Bansil et al PRB(2005)

Hubbard interaction (left): $U = -1.2 \rightarrow 0.52eV$

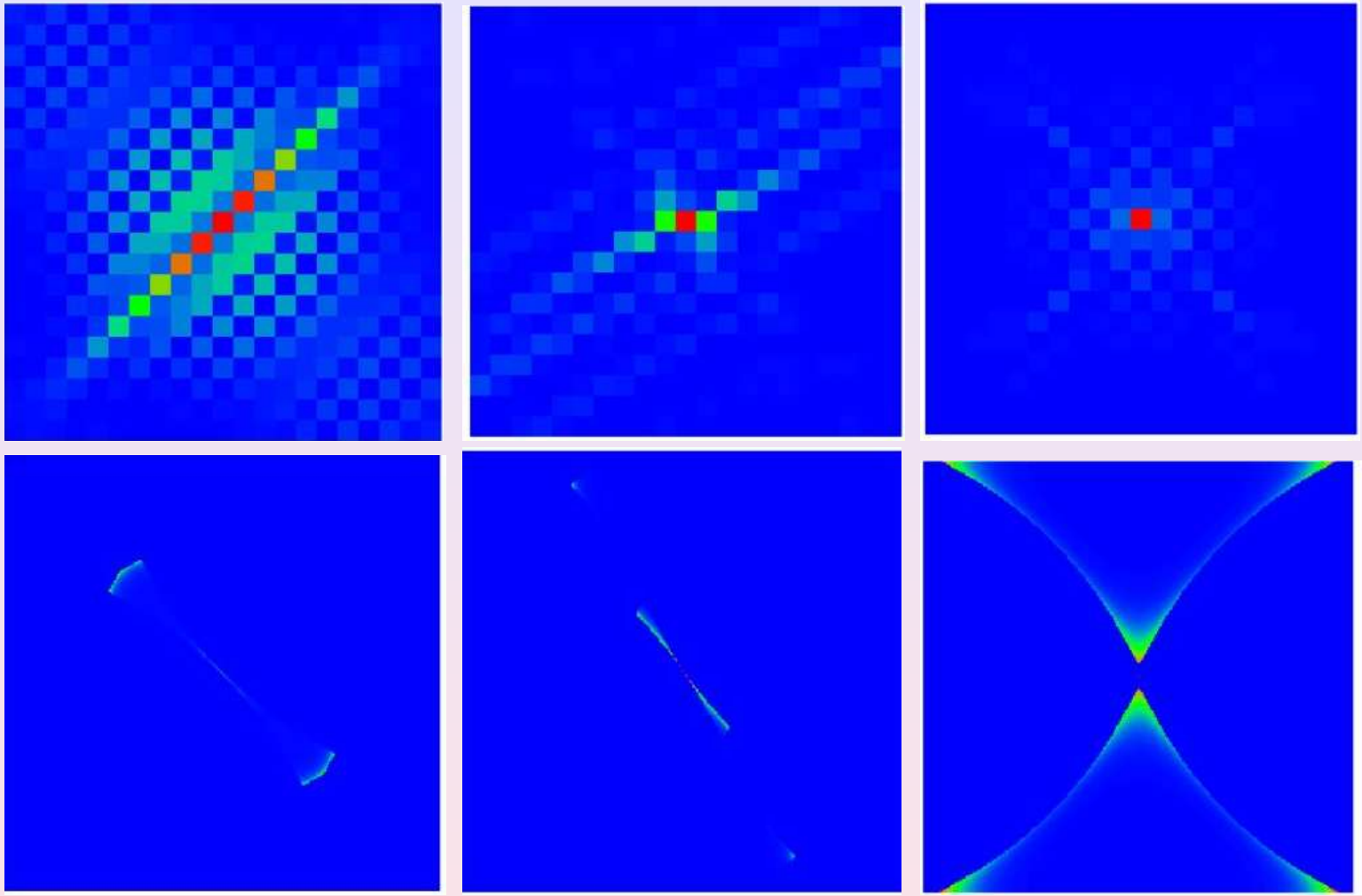
d-wave interaction (right): $U = -2 \rightarrow 0.86eV$

Mobile hole pairs: energy landscape



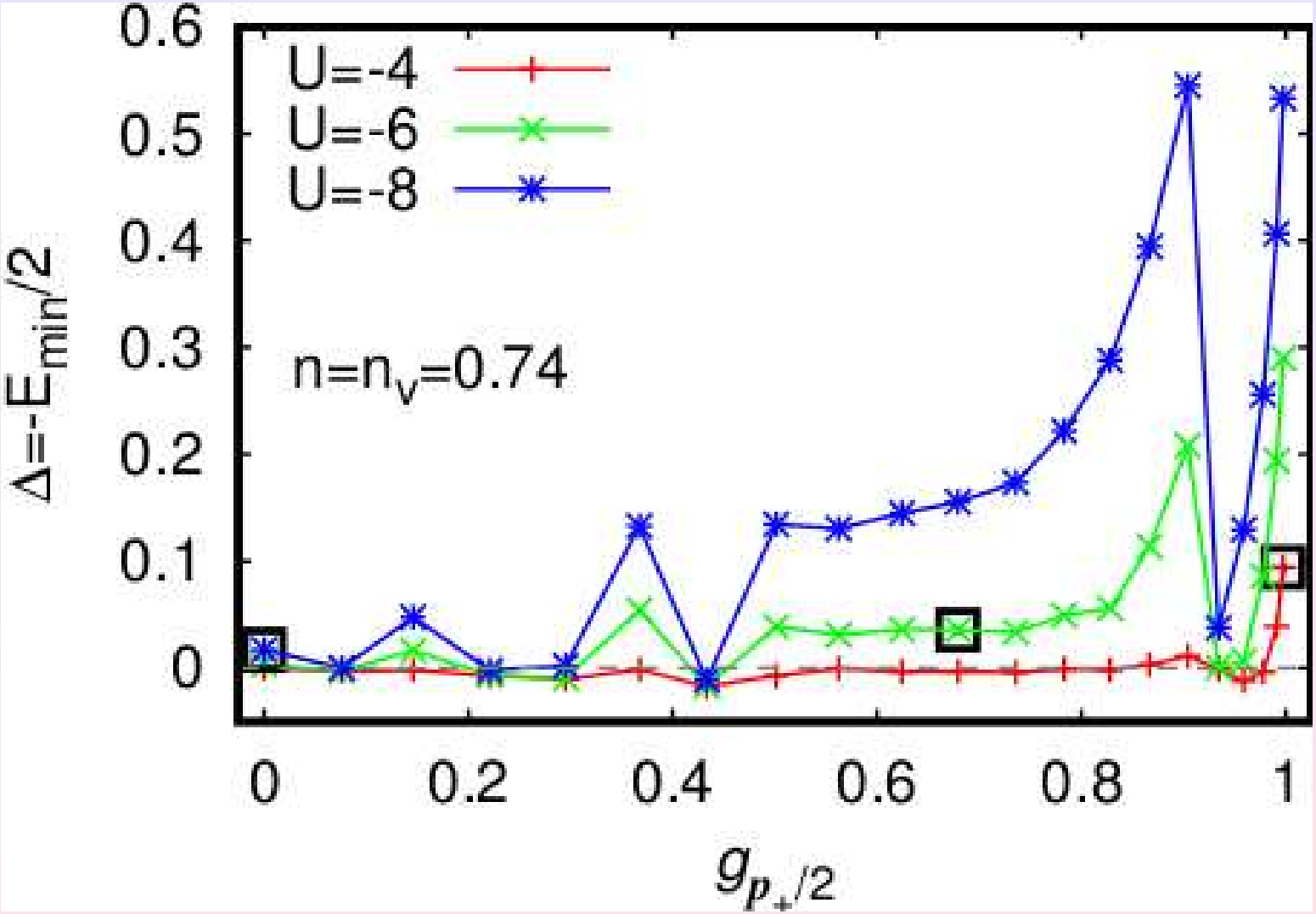
Dopping $n_h = 1 - n = 1 - 0.74 = 0.26$, virtual filling $n_v = n$ ($p_{x,y} = p_{+x,+y}/2$);
$p_{+x,+y} = 2\pi(103, 103)/256$ (left - node), $2\pi(46, 172)/256$ (center),
$2\pi(0, 248)/256$ (right - antinode) BOTTOM panels: frozen Fermi sea effect

Mobile hole pairs: ground states



Top: coordinate space (zoom (-10,10)); bottom: momentum space $(-\pi, \pi)$;
Hubbard: $U = -8, \Delta = -0.034/2$ (left - node); $U = -6, \Delta = -0.071/2$ (center); $U = -4, \Delta = -0.18/2$ (right - antinode);
other parameters as in previous slide; $N = 256$

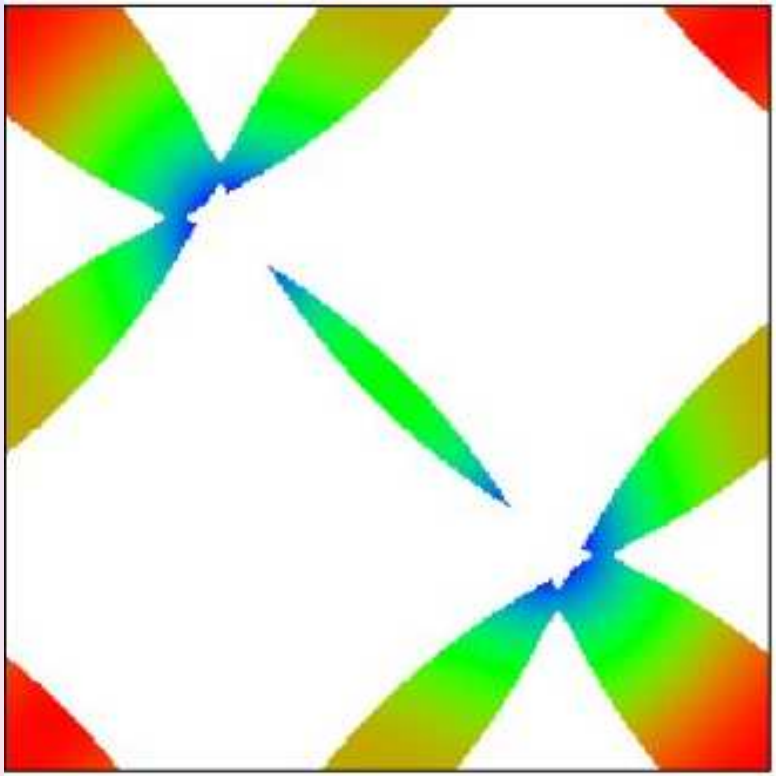
Gap for mobile hole pairs

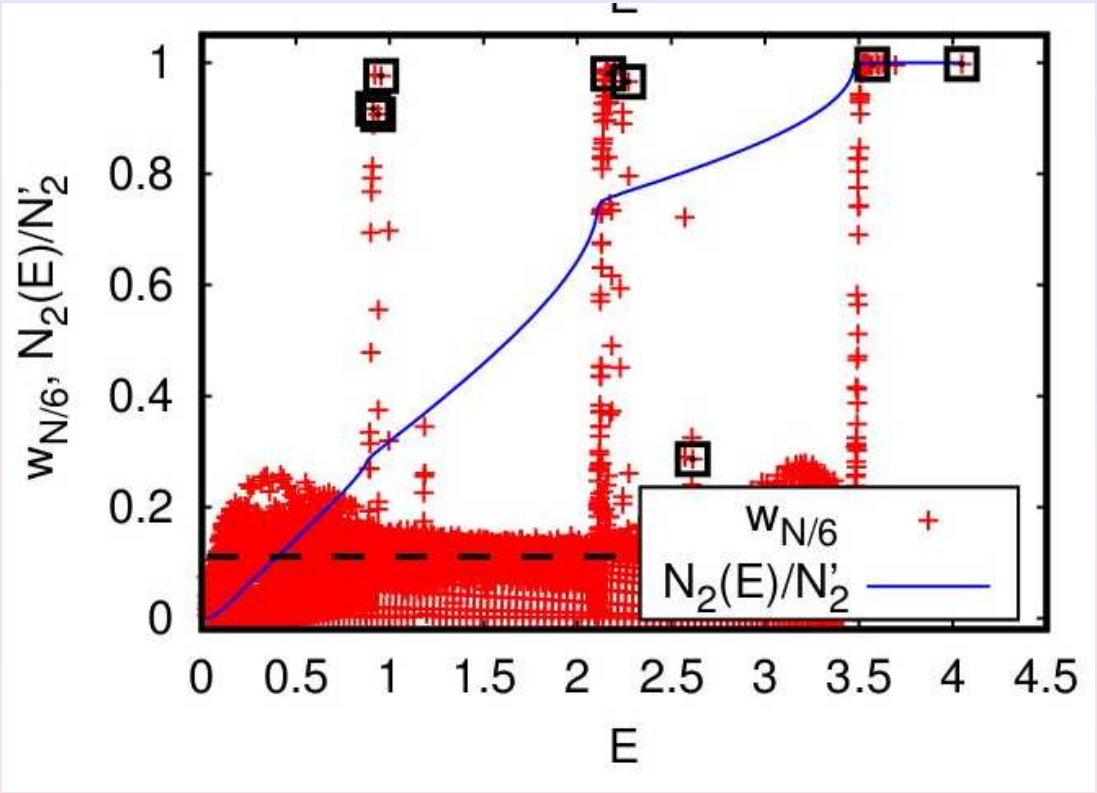


Mobile hole pairs at $n_h = 1 - n = 0.26$, $n_v = n$, Hubbard

$g_{p_+/2} = [\cos(p_{+x}/2) - \cos(p_{+y}/2)]/2$

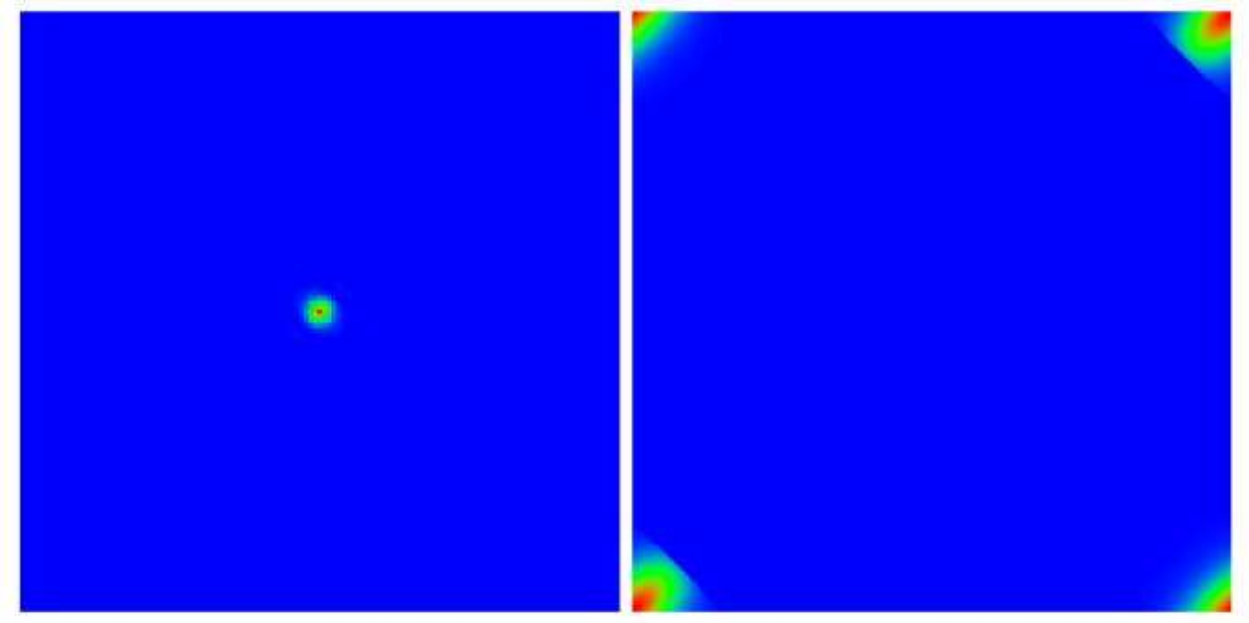
Coulomb mobile pairs (electrons)





Mobile electron pairs at $n = 0.74$, $n_v = 1$, $U = 2$, $p_{+x,+y} = 2\pi(113, 113)/256$, $N = 256$; left: energy landscape, right: pair probability $W_{N/6}$ (red +) (level number N_2/N_2' - blue curve) vs energy above Fermi level E

Coulomb mobile pairs (electrons)



Mobile electron pair at $n = 0.74, n_v = 1, U = 2, p_{+x,+y} = 2\pi(113, 113)/256$,
left: coordinate space, right: momentum space, $N = 256$
3 mechanisms of Coulomb pair formation:
* - narrow (flat band),
* - local negative mass at energy landscape,
* - location in small accessible islands above frozen Fermi sea

Discussion

* - Formation of static Cooper pairs in LSCO by
attractive Hubbard (s-wave) and d-wave interactions:
very similar ground state structure;
d-wave features even for Hubbard case due to Fermi surface structure

* - Gap and T_c dependence on hole dopping is close to
experimental LSCO data both for Hubbard and d-wave interactions

* - Mobile Cooper pairs: unusual energy landscape due to frozen Fermi sea;
gap appears at stronger attraction compared to static pairs;
possible link between mobile pairs and stripes

* - Three mechanisms for pair formation by Coulomb repulsion above Fermi level; no gap found