Variational Cluster Approach to the Bilayer Hubbard Model

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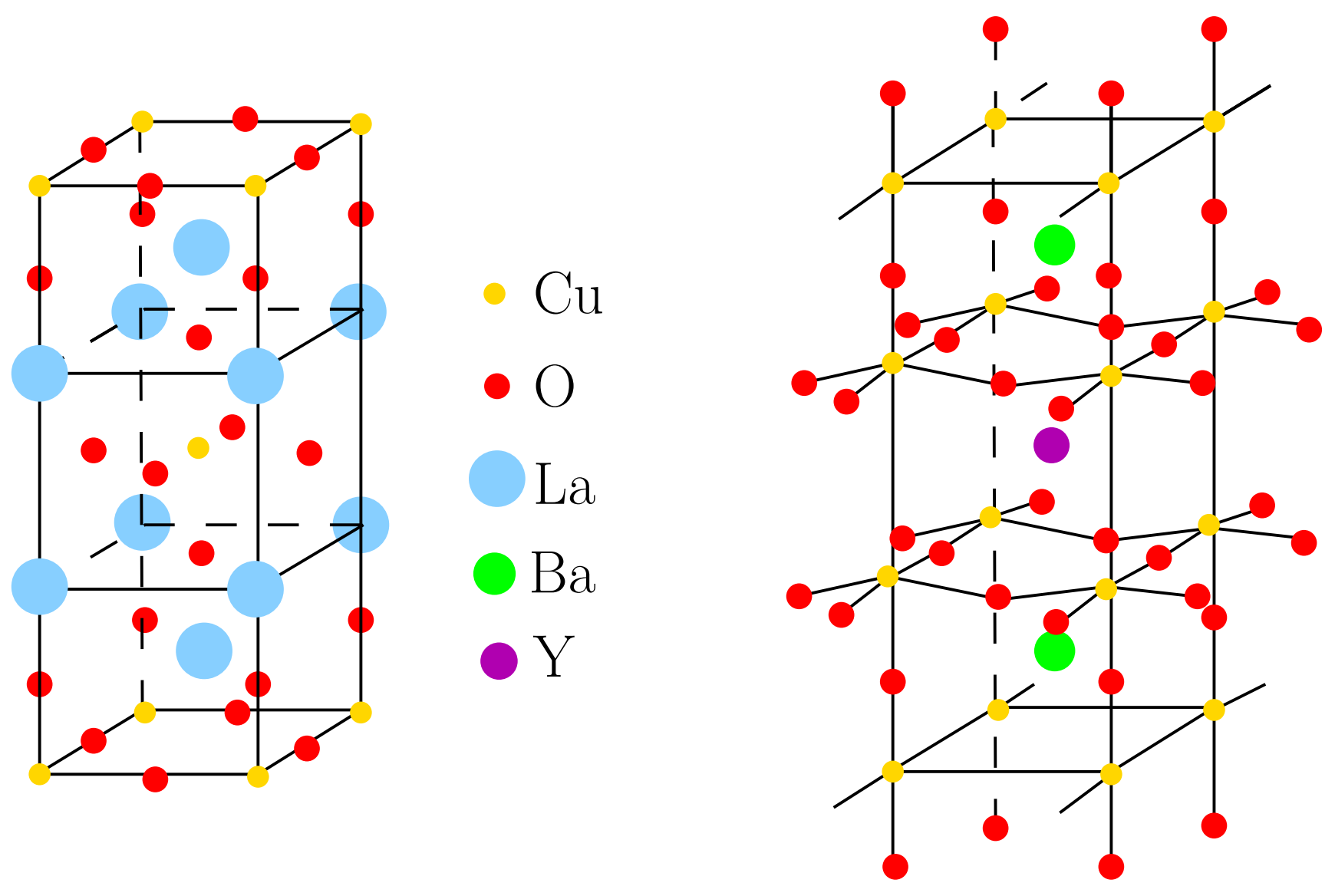
Bilayer High Temperature Superconducting Cuprates

- HTSC have perovskite structure
- superconductivity occurs in $\mathbf{CuO}_2$ layers
- most HTSC contain two ore more $\mathbf{CuO}_2$ layers next to each other
- the interlayer hopping is expected to influence the critical temperature and doping dependence of superconductivity.
- ARPES experiments [1] show a bilayer splitting in the spectral functions of hole doped Bi2212, which is reduced from 88 meV in the normal state to 20 meV superconducting state.

$$\Longrightarrow$$

- use the Hubbard Model to describe a $\mathbf{CuO}_2$ layer
- Variational Cluster Approach (VCA) ([2],[3]) to study phase diagram and spectral functions at different doping levels with and without interlayer hopping
- measure bilayer splitting



LaCuO (monolayer)　YBCO (bilayer)

Model

- Hubbard Hamiltonian (one layer)

$$H_H = -t \sum_{\langle ij\rangle,\sigma} (c^{+}_{i\sigma} c_{j\sigma} + c^{+}_{j\sigma} c_{i\sigma}) + t' \sum_{\langle\langle ij\rangle\rangle,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \mu \sum_{i\sigma} n_{i\sigma} \quad (1)$$

- Interlayer hopping (in momentum space)[4]

$$H_{inter} = \sum_{k,\sigma} t_{\perp} \frac{v^2}{(1-2u\frac{t'}{t})^2} (c^{\dagger}_{k\sigma a} c_{k\sigma b} + c^{\dagger}_{k\sigma b} c_{k\sigma a}) \quad (2)$$

with $u = (\cos(k_x) + \cos(k_y))/2$ and $v = (\cos(k_x) - \cos(k_y))/2$, while a and b denote the layers. For $t'/t << 1$ it follows that $H_{inter} \approx \sum_{k,\sigma} t_{\perp} v^2 (c^{\dagger}_{k\sigma a} c_{k\sigma b} + c^{\dagger}_{k\sigma b} c_{k\sigma a})$.

In real space this corresponds to

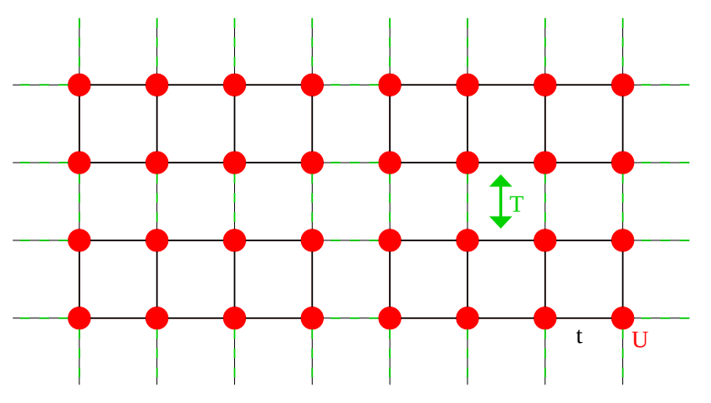
$\sum_{\Delta x,\Delta y,\sigma} \frac{t_{\perp}}{4} \left(\delta_{\Delta x,0}\delta_{\Delta y,0} - \frac{1}{2}\delta_{\Delta x,\pm 1}\delta_{\Delta y,\pm 1} + \frac{1}{4}\delta_{\Delta x,0,\pm 2}\delta_{\Delta y,0,\pm 2}\right) (c^{\dagger}_{i+(\Delta x,\Delta y)b\sigma} c_{ia\sigma} + h.c.)$.

Parameters

U	$8t$
t'	$0.3t$
$t_{\perp}$	$-0.4t$

We have chosen $t_{\perp} = -0.4t$.
[4] get for YBCO $t_{\perp} \approx -0.625t$ and [5] use $t_{\perp} = -0.3t$ for BSC0.

Solver: Variational Cluster Approach



CPT:

$$H = H_{\mathbf{CL}} + H_{\mathbf{intercl}}$$

$$G^{-1}_{\mathbf{CPT}} = G^{-1}_{\mathbf{CL}} - T$$

- Exact diagonalization of the cluster Hamiltonian using the Lanczos procedure. (4x2x1 sites)
- Intercluster hoppings, including $t_{\perp}$, treated perturbatively (CPT,[6]).
- Variational calculation to allow symmetry-broken phases ([3],[2],[7]):

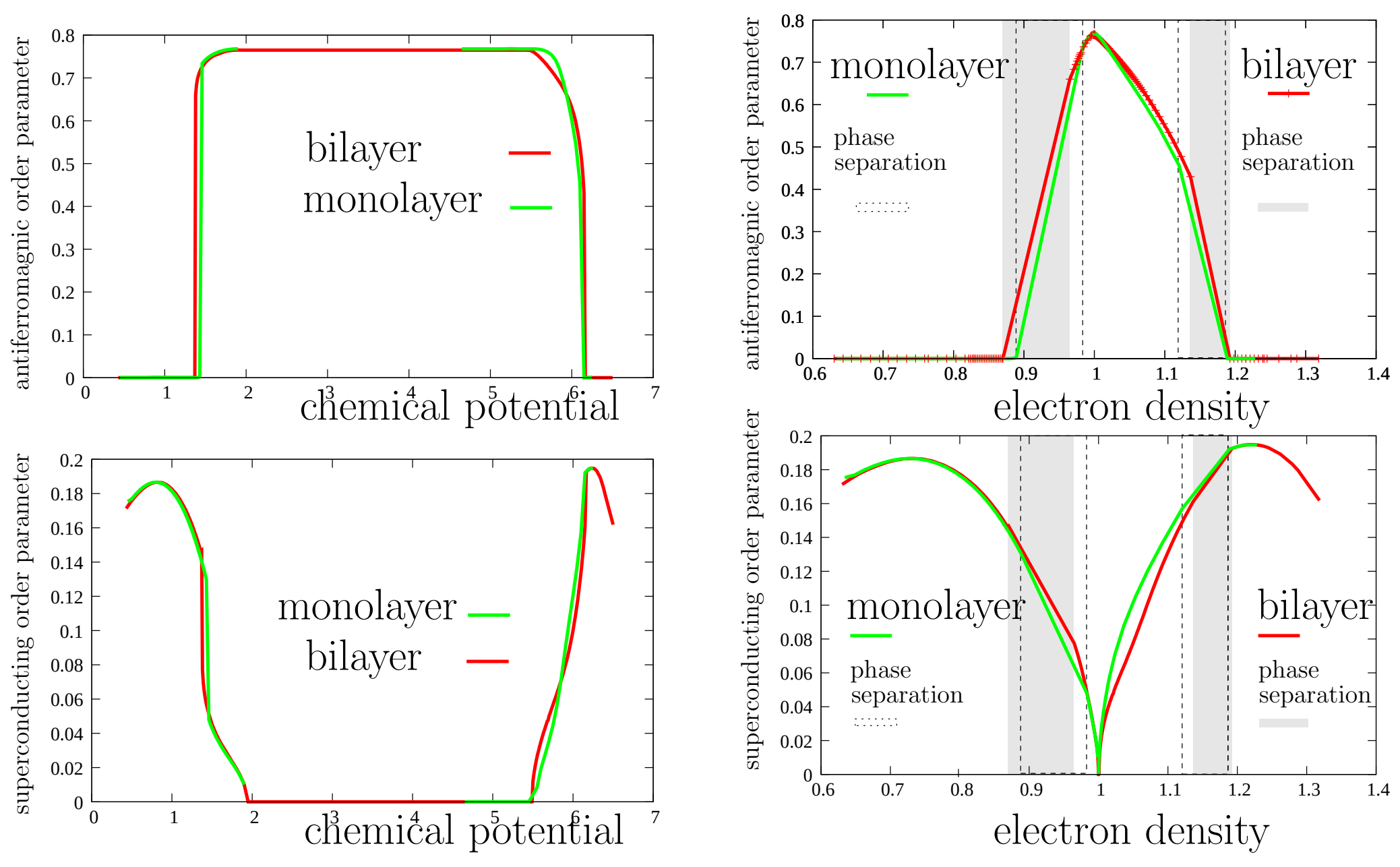
$$H'_{\mathbf{CL}} = H_{\mathbf{CL}} + h_{field} \qquad H'_{\mathbf{intercl}} = H_{\mathbf{intercl}} - h_{field}$$

with

$$h_{field} = h_{SC} \sum_{i,j} \frac{\eta_{i,j}}{2} (c_{i,\uparrow} c_{j,\downarrow} + h.c.) + h_M \sum_{i\sigma} (-1)^{\sigma} e^{i\mathbf{Qr}} c^{\dagger}_{i,\sigma} c_{i,\sigma} \quad (3)$$

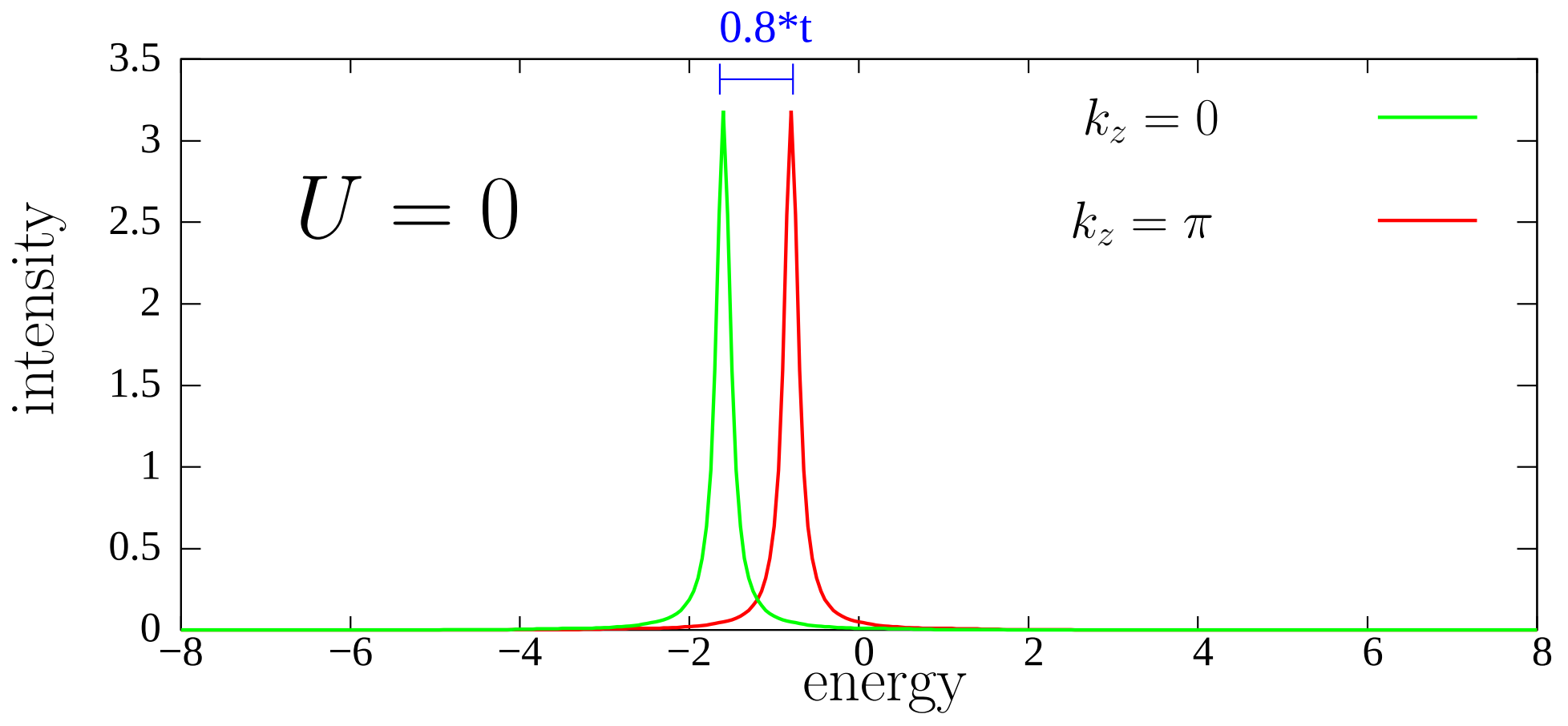
Results - Phase Diagram

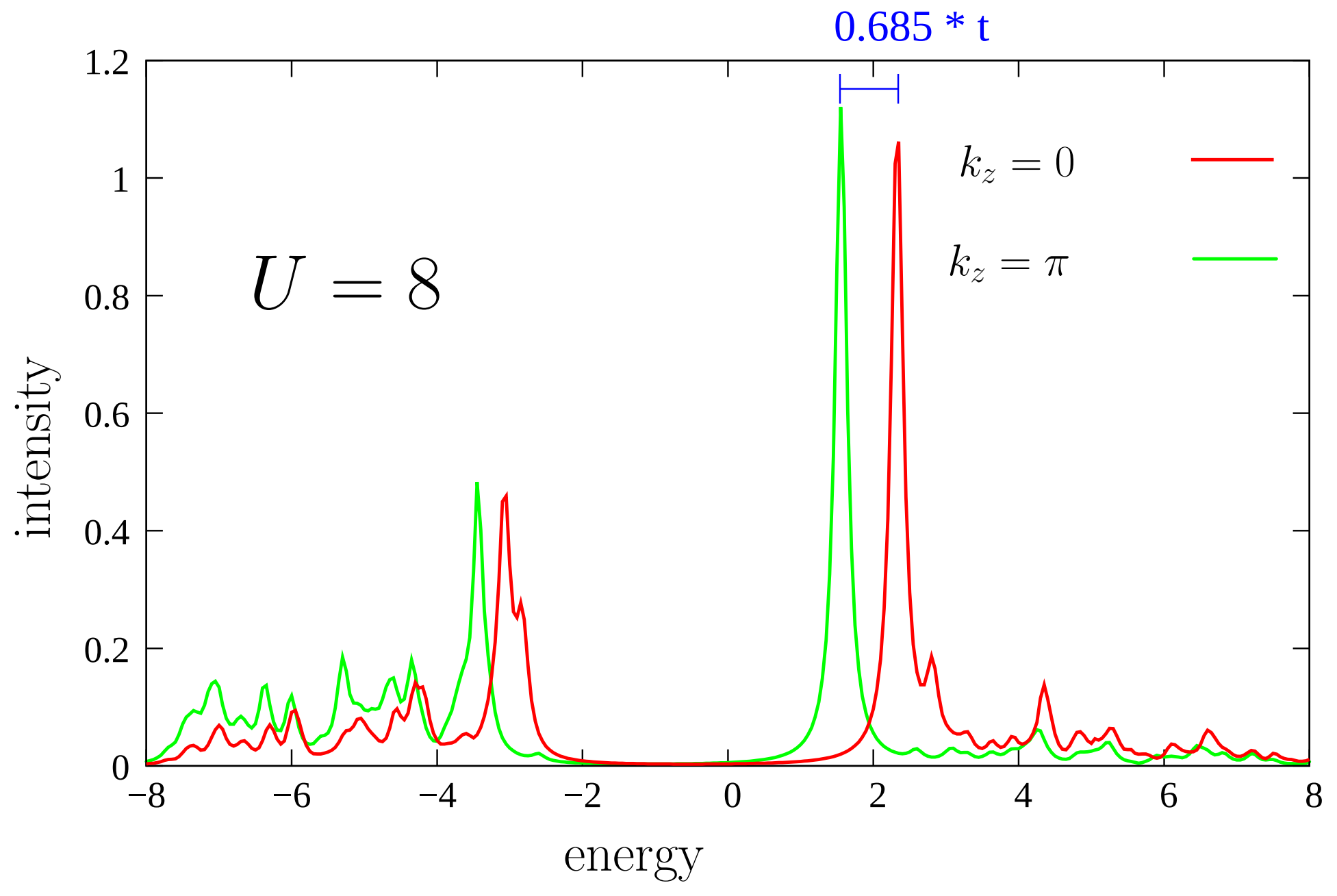
- very similar to mono-layer phase diagram
- antiferromagnic zone around half filling([8],[9],[10])
- at electron and hole doping a d-superconducting phase forms
- critical doping for superconductivity is different for electron and hole doping, as well as the vanishing of the antiferromagnic phase.
- optimal doping is overestimated in size



Bilayer Splitting at Half Filling

Density of states (DOS) at the point of maximum splitting $(0,\pi)$, for correlation $U = 0$ and $U = 8$.

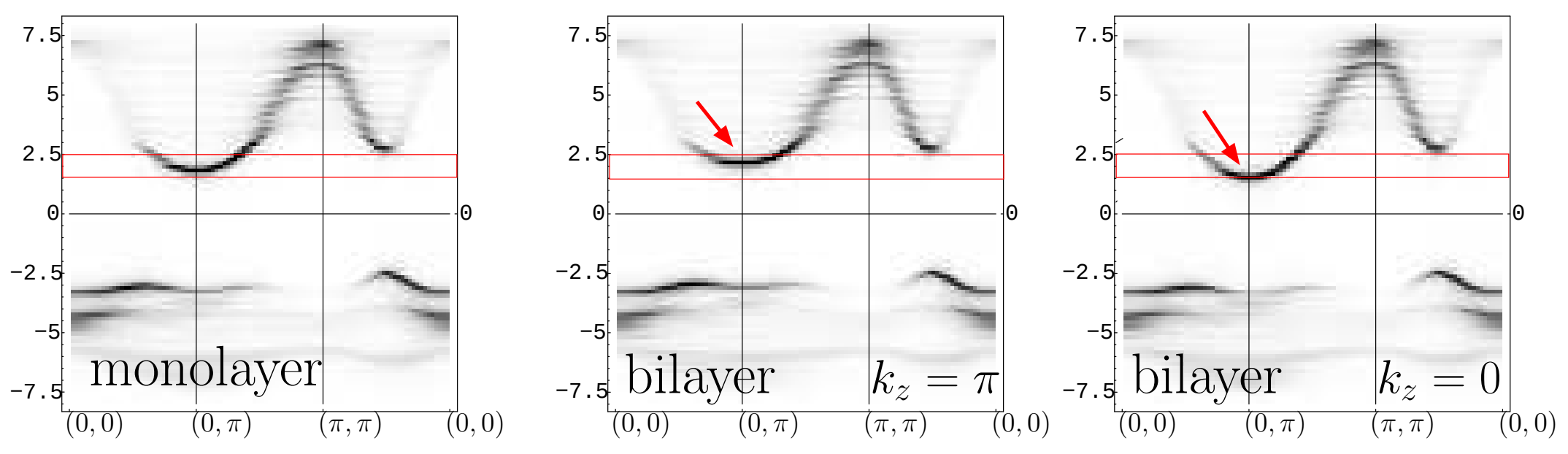




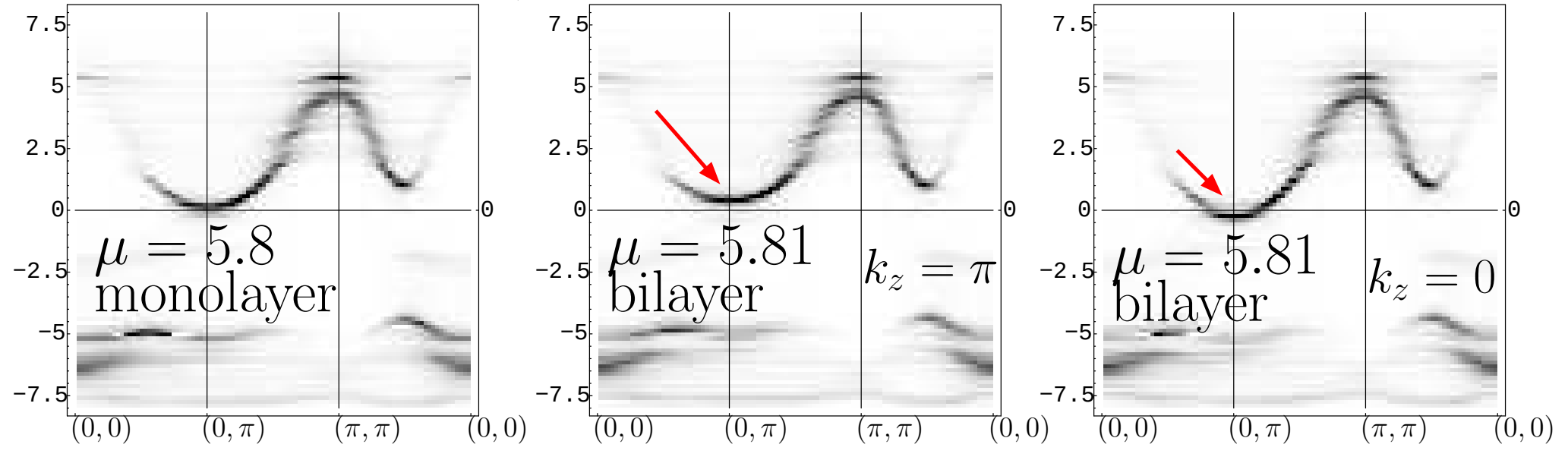
For $U = 0$ there is one exitation for $k_z = 0$ and $k_z = \pi$ each, with a splitting of $\Delta E(0,\pi) = 0.8t$.
For $U = 8$ the DOS is gapped and the splitting is reduced to approximately $\Delta E(0,\pi) = 0.685t$.

Results - Spectral Function

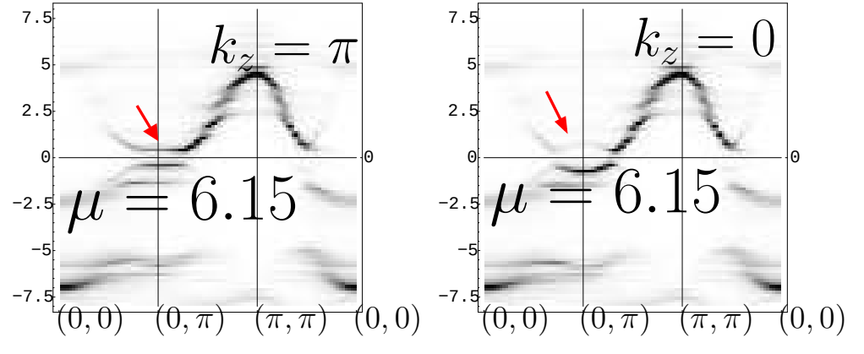
The spectral functions at half filling for monolayer and bilayer $(k_z = 0, k_z = \pi)$ case:



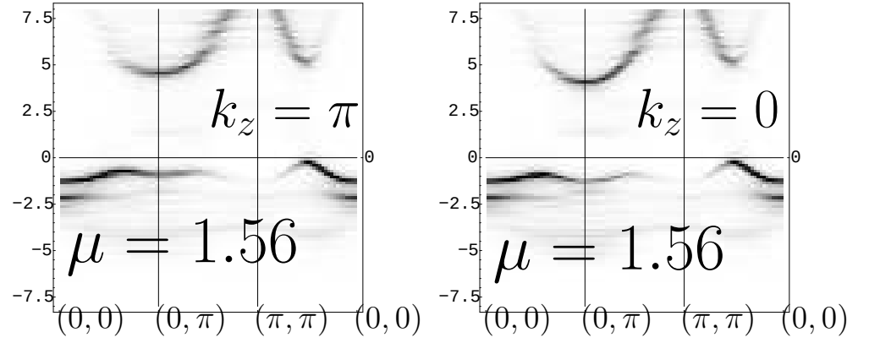
The spectral functions at electron doping (which in nature was not found for bilayer HTS), bilayer $n = 1.074$, monolayer $n = 1.03$:



Electron doping $n = 1.272$

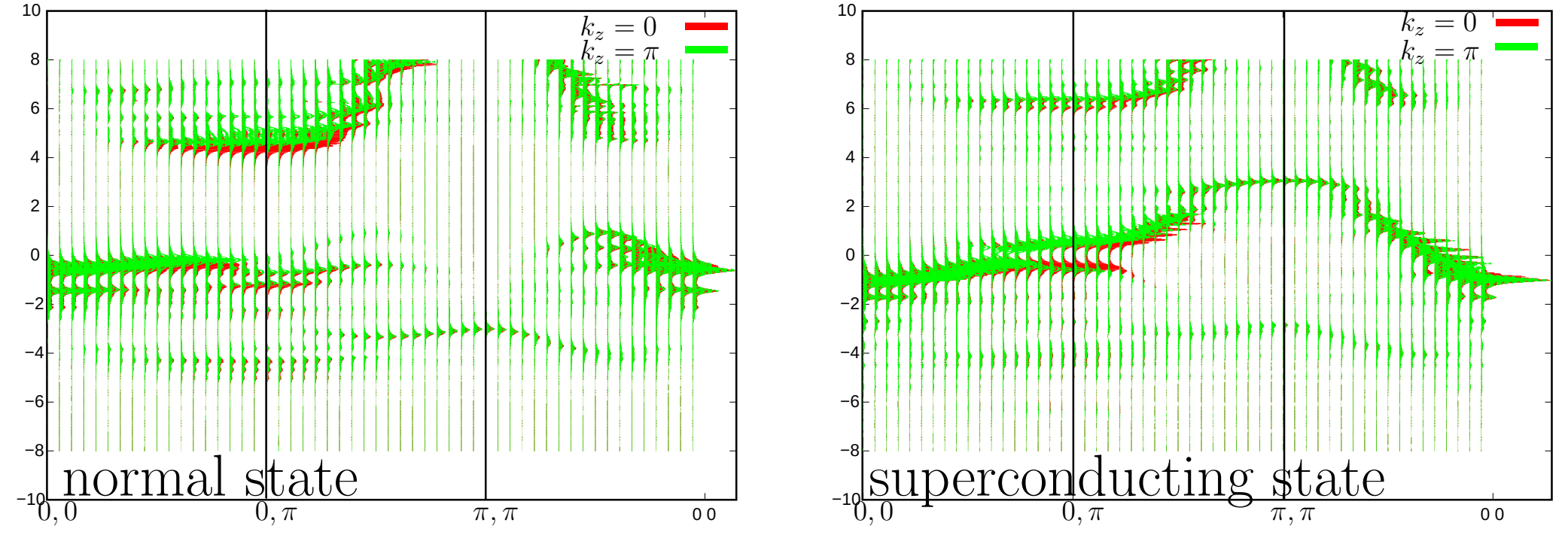


Hole doping $n = 0.973$



Heavily Overdoped (With Holes)

- ARPES measurements on Bi2212 [1] indicate that the splitting is reduced in the superconducting case.
- $\Rightarrow$ calculate the spectral function of the highly overdoped bilayer system both in the normal and superconducting state

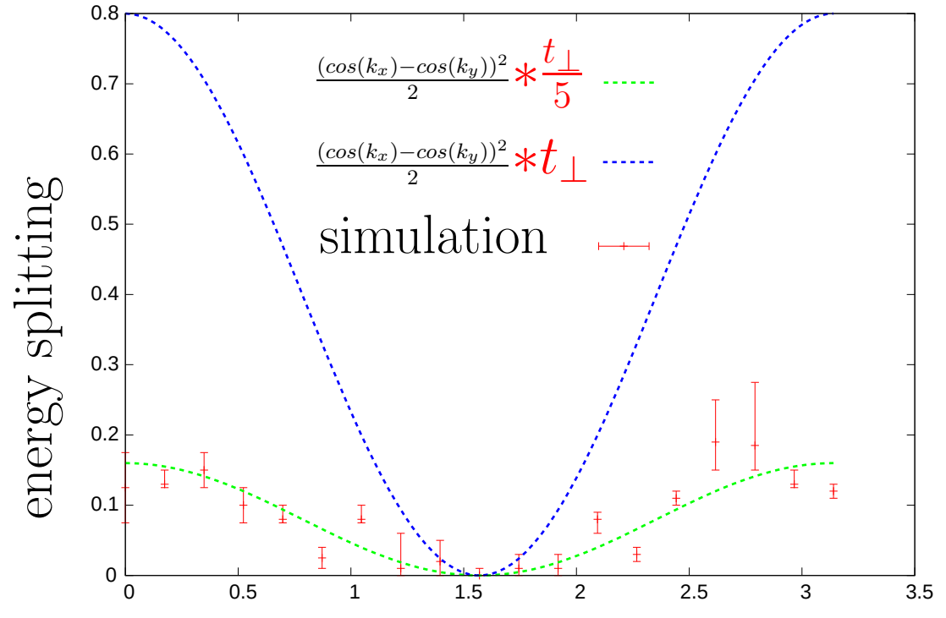


- compare bilayer splitting on the $\mathbf{k} = (0,\pi)$ to $\mathbf{k} = (\pi,0)$ line of the Brillouin Zone for superconducting state and normal state with the values

$$\Delta E = \frac{(cos(k_x) - cos(k_y))^2}{2} t_{\perp} \quad (4)$$

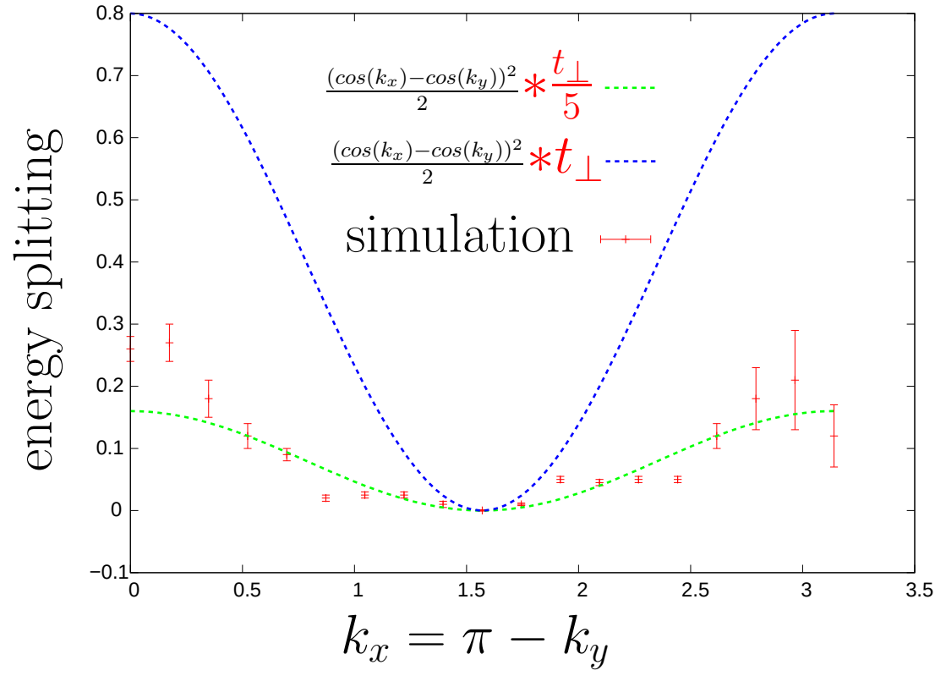
(blue line in figures), expected without correlation ($U = 0$).

superconducting state:



The curve that describes the bilayer splitting for $U = 0$ is fitted to the values obtained with VCA calculation (red points with errorbars). Multiplication with a factor $\frac{1}{5}$ (green line) fits the data both in the superconducting and normal case quite well.

normal state:



$\Rightarrow t_{\perp}$ is renormalized to about $\frac{t_{\perp}}{5}$. Around $\mathbf{k} = (0,\pi)$ the bilayer splitting seems to be about twice the size in normal state, compared to the superconducting state.

Conclusions

The interlayer hopping

- introduces differences in the phase diagram between the monolayer and bilayer Hubbard model
- causes a splitting of the energy bands.

Comparison of the energy splitting for

$U = 0$

- all bands split according to

$$t_{\perp} \frac{(\cos(k_x) - cos(k_y)^2)}{2}$$

  - the bands lie exactly onto each other at the Brillouin Zone diagonal $k_x = k_y$,
  - maximal splitting at the $(0,\pi)$ and $(\pi,0)$ points
- maximum splitting amounts to $\Delta E(0,\pi) = 0.8t = 2t_{\perp}$

$U = 8$

- Splitting of the bands has the same form but renormalized $t_{\perp}$
- heavily overdoped sample, superconducting state $\Delta E(0,\pi) \approx (0.15 \pm 0.05)t \approx 0.375t_{\perp}$
- heavily overdoped sample, normal state $\Delta E(0,\pi) \approx (0.26 \pm 0.04)t \approx 0.65t_{\perp}$
- half filling (antiferromagnic state) $\Delta E(0,\pi) \approx 0.685t = 1.7125t_{\perp}$.

At $\mathbf{k} = (0,\pi)$ we see a decrease in bilayer splitting from normal to superconducting state of about 50%, which is much less then what obtained within experiment [1]

References

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