An $SU(2)$ Approach to the Pseudogap Phase of Cuprates

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We use an $SU(2)$ mean-field theory approach with input from variational wave functions of the t-J model to study the photoemission spectra of cuprates in the pseudogap phase. In our model, the pseudogap state of underdoped cuprates is realized by classical fluctuations of the order parameter between the d-wave superconductor and the staggered-flux state. Spectral functions of the intermediate and the averaged states are computed and analyzed. We find that the photoemission spectrum shows an asymmetric gap structure interpolating between the superconducting gap centered at the Fermi energy and the asymmetric staggered-flux gap. Our model predicts that this asymmetry changes sign at the point where the Fermi surface crosses the diagonal $(\pi,0)$-$(0,\pi)$.

Introduction

An approximate symmetry for lightly doped projected wavefunctions

A minimal model for cuprate layers - the t-J Hamiltonian:

$$H_{t\text{-}J} = P_d[-\sum_{i,j,\sigma} t_{ij}\, c^\dagger_{i,\sigma} c_{j,\sigma} + J\sum_{\langle i,j\rangle}(\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \frac{n_i n_j}{4})]P_d\,.$$

Consider the local transformation of the fermion doublet $\boldsymbol{\psi}^\dagger = (c^\dagger_\uparrow, c_\downarrow)$:

$$\psi \to g\psi \qquad (1)$$

where $g \in SU(2)$.

The operator $\boldsymbol{S} = \frac{1}{2}c^\dagger_\alpha \boldsymbol{\sigma}_{\alpha\beta} c_\beta$ is invariant under transformation (1). Therefore, when $x \to 0$ (half filling), the t-J model has a local $SU(2)$ symmetry [1, 2].

Consider the (variational) wave function

$$|\varphi\rangle = P_d\,|\varphi_0\rangle$$

where $|\varphi_0\rangle$ is an eigenstate of some auxiliary mean-field Hamiltonian

$$H^U_{MF} = \sum_{ij}\boldsymbol{\psi}^\dagger_i U_{ij}\boldsymbol{\psi}_j - \mu\sum_i \boldsymbol{\psi}^\dagger_i\sigma_3\boldsymbol{\psi}_i\,.$$

At half-filling ($\mu = 0$), the family of mean-field Hamiltonians, connected by $SU(2)$ rotations,

$$\tilde{H}^U_{MF}[g] = H^{\tilde{U}}_{MF}$$

where $\tilde{U}_{ij} = g^\dagger_i U_{ij} g_j$, provide identical wavefunctions for the t-J model. At small doping, the different states are split in energy. By continuity, the splitting is expected to be small. This provides a route to construct a host of low-energy states for the lightly doped t-J model [3].

The variational theory of high-Tc cuprate superconductors

The variational approach predicts a d-wave superconductor (SC) as the most competitive ground state of the doped t-J model on the square lattice [4, 5]:

$$U^{SC}_{jk} = -\chi\sigma_3 + i(-)^{j_x+k_x}\Delta\,\sigma_1.$$

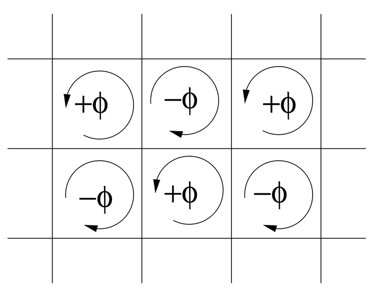
The projected d-wave ground state wavefunction and low-lying quasiparticle (QP) excitations reproduce many experimental observations in the superconducting state of HTSC (gap symmetry, SC dome, nodal velocities, spectral weights, QP current, etc.) [6, 7, 8, 9, 10].

Vortex cores in the underdoped region

In the case of HTSC, conventional $U(1)$ vortices are very costly in energy (large gap). "Cheap"vortices with *staggered-flux* (SF) normal cores may be constructed using a staggered $SU(2)$ rotation [3]:

$$U^{SF}_{jk} = g^\dagger_j U^{SC}_{jk} g_k$$

and $g_j = e^{i\frac{\pi}{4}(-)^j\sigma_1}$. The SF is a mean-field state with staggered magnetic fluxes, $\phi = 4\arctan(\Delta/\chi)$, through the plaquettes:



$$U^{SF}_{jk} = -\chi\sigma_3 - i\Delta(-)^{j_x+k_y}$$

Intermediate states between SF and SC

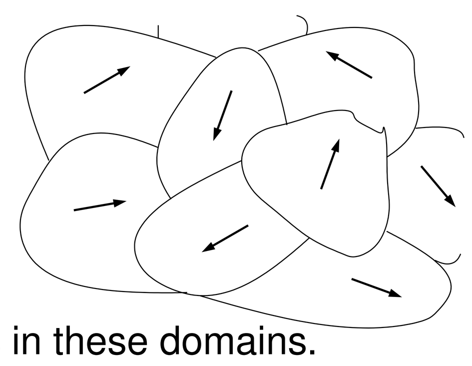
In general, the $SU(2)$ rotations at every site can be parametrized by three Euler angles,

$$g = e^{i\frac{\alpha}{2}\sigma_3}e^{i\frac{\theta}{2}\sigma_1}e^{i\frac{\varphi}{2}\sigma_3}.$$

α is the $U(1)$ phase of the electron. A point on the sphere parameterized by (θ,φ) represents a particular mean-field state. Staggered rotations $\theta_j = \frac{\theta}{2}(-1)^j$ interpolate between the SC state (equator; $\theta = 0$) and the SF state (north and south poles, $\theta = \pm\frac{\pi}{2}$). The vortex is a (half-)hedgehog on this sphere [11, 12].

The Model

We are in interested in the photoemission spectra (ARPES) for the underdoped region, when large variations of the order parameter occur. We model those variations by domains with constant g and disregard short-wavelength α and φ fluctuations in these domains.



Hamiltonian for a domain

In a given domain of the sample, the effective Hamiltonian is

$$H_{MF}(\Delta,\theta) = \sum_{\langle i,j\rangle}\boldsymbol{\psi}^\dagger_i g^\dagger_i(\theta)U^{SC}_{ij}(\Delta)g_j(\theta)\boldsymbol{\psi}_j - \chi'\sum_{\langle\langle i,j\rangle\rangle}\boldsymbol{\psi}^\dagger_i\sigma_3\boldsymbol{\psi}_j - \mu\sum_i\boldsymbol{\psi}^\dagger_i\sigma_3\boldsymbol{\psi}_i\,.$$

with $g_j = e^{i(-)^j\frac{\theta}{2}\sigma_1}$.
The chemical potential is used to fix the fermion number. An additional next-n.n. hopping χ' (unrotated; $\chi' \simeq -0.3\chi$) is introduced on a phenomenological basis (geometry of experimental Fermi surface; results of exact Gutzwiller projection [9]).

The one-particle spectral function is relevant for ARPES experiments. We compute it for the effective Hamiltonian parameterized by (Δ,θ),

$$A^{(\Delta_\theta,\theta)}_{\mathbf{k},\omega} = -\frac{1}{\pi}\mathrm{Im}G_{\mathbf{k}}(\omega + i\Gamma)\,.$$

This (unprojected) model is viewed as an effective model for projected quasiparticle excitations [8, 13]. Parameters are taken from variational computations in the t-J model (for $t = 3J$): $\Delta_0 \simeq 0.25\chi$, $\Delta_{\pi/2} \simeq 0.2\chi$, $\chi \simeq 0.3t$ at $x \simeq 10\%$ (holedoping).

Averaged Green's function

In general, one would compute

$$\langle A_{\mathbf{k},\omega}\rangle = Z^{-1}\int D\tilde{U}A^{\tilde{U}}_{\mathbf{k},\omega}e^{-\beta E[\tilde{U}]}$$

where the free energy $E[\tilde{U}]$ is flat in directions parameterized by g, $\tilde{U} = g^\dagger U g$.

We consider the case:

- restriction to g interpolating between SF and SC states (U^{SC}).
- slow spatial variations of the order parameter (domains of constant g).
- sufficiently high temperature such that we can neglect the dependency of the free energy on g (Variational Monte Carlo predicts $\varepsilon_c = E^{SF} - E^{SC} \simeq 0.02J$ per site [13]).
- negligible amplitude fluctuations in U (or Δ; the corresponding energy scale is large, of order T^*).

In this situation, the averaged spectral function is given by

$$\langle A_{\mathbf{k},\omega}\rangle = \tilde{Z}^{-1}\int d\cos\theta\, A^{(\theta,\Delta_\theta)}_{\mathbf{k},\omega}$$

Results

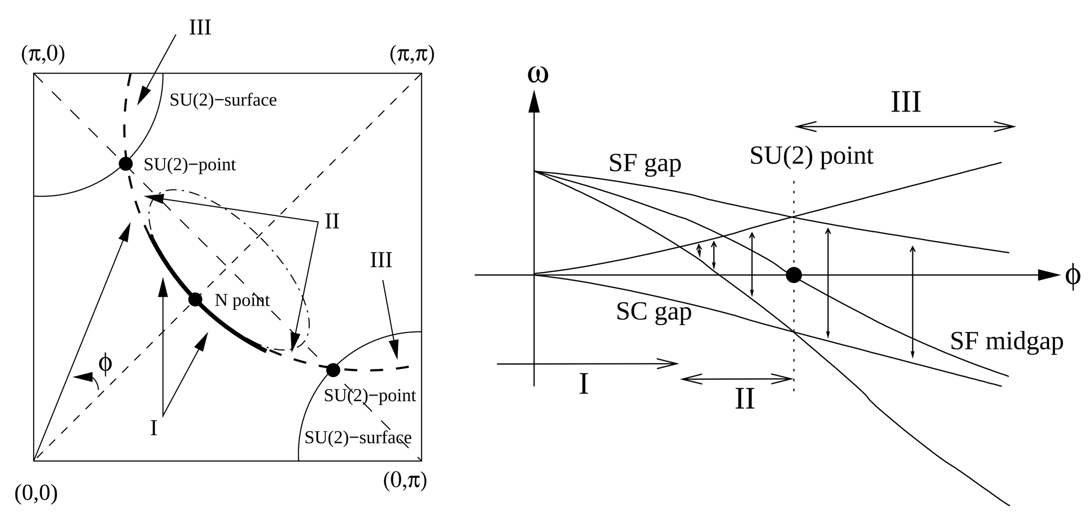


Abbildung 1: Schema of the different regions of the Fermi surface. Left: first BZ with SC (- -) and SF (-.-) Fermi surfaces. Right: four bands which evolve into one another as θ is increased from 0 (SC) to $\pi/2$ (SF).

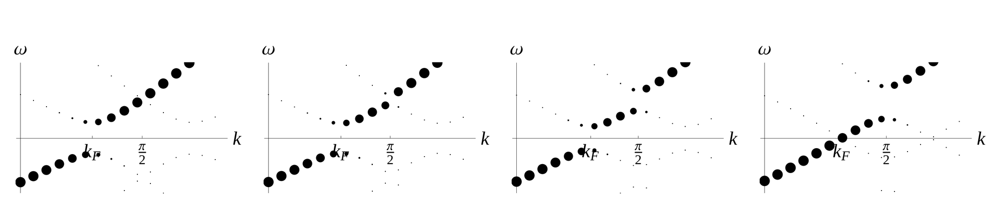


Abbildung 2: Schematic evolution of the spectrum along a cut parallel to the nodal direction, inside the pocket (through region I in Abbildung 1). From L to R: $\sin\theta = 0, 1/3, 2/3, 1$. Left corresponds to the SC state, right to the SF state. The SC gap opens on the SC Fermi surface, the SF gap on the diagonal $(0,\pi)$-$(\pi,0)$.

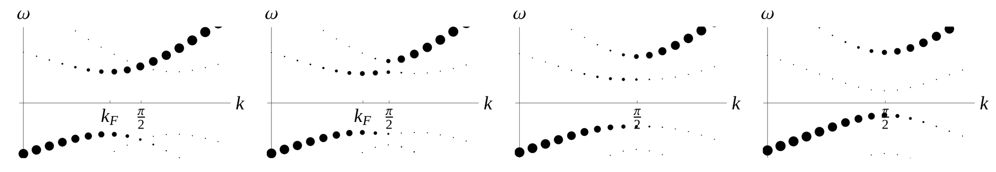


Abbildung 3: Same plot as Abbildung 2, but for a cut outside the pocket (through region II in Abbildung 1).

- Discussion of Abbildung 1: the Fermi surface appears as a (nearly) gapless arc in region I (depending on the definition of the effective gap and the QP lifetime). In region II, the staggered-flux gap and the superconducting gap start to overlap and form an effective gap which is shifted towards positive energy (vertical arrows on right plot). The effective gap comes down in energy as we go towards the antinode in region II. Exactly at the $SU(2)$-points on the diagonal $(0,\pi)$-$(\pi,0)$, the effective gap is symmetric. Beyond the $SU(2)$-points (region III), the midgap is shifted below the Fermi energy.

At the $SU(2)$-points [more generally, at the $SU(2)$ surface where $\mu + 2\chi'\cos k_x\cos k_y = 0$], the full $SU(2)$ symmetry is intact even away from half-filling; the spectral functions are independent of θ [if we neglect the weak dependency $\Delta(\theta)$].

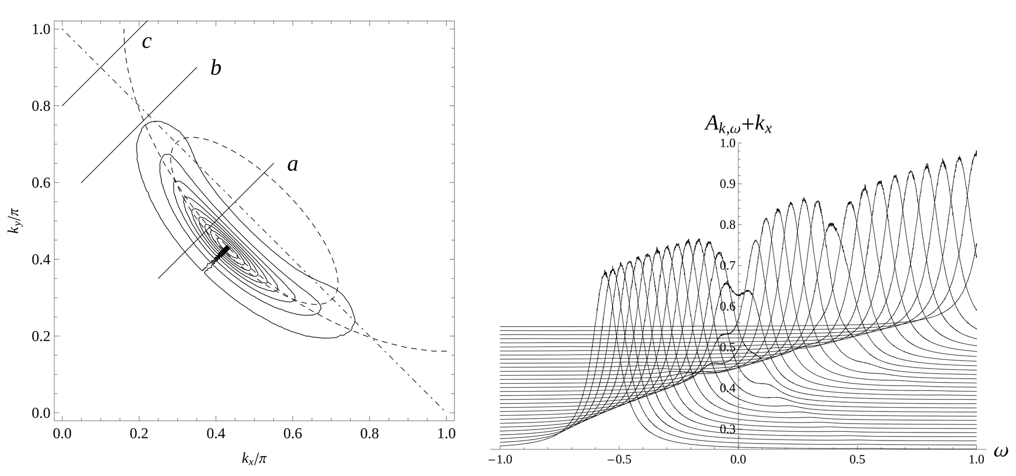


Abbildung 4: left: averaged spectral function at the Fermi energy, $A_{\mathbf{k},\omega=0}$. Right: spectral function on cut a. The SF and SC gaps are washed out by the averaging and an almost gapless arc appears.

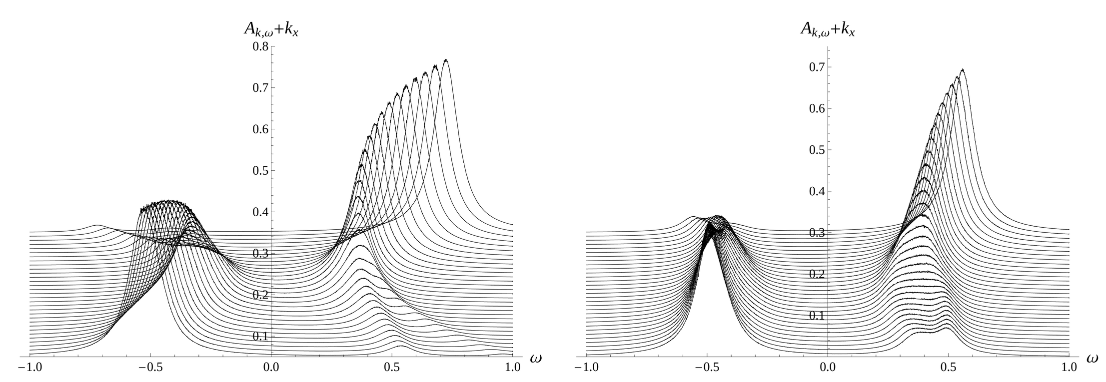


Abbildung 5: left: averaged spectral function on cut b. The effective gap is shifted to positive energy. Right: averaged spectral function on cut c. The effective gap is shifted to negative energy. (Energy units are $2\chi \simeq 200\,\mathrm{meV}$. QP lifetime $\Gamma = 0.12\chi$)

Experimental implications

The most striking prediction of our model, the suppression of intensity due to formation of a staggered-flux gap above the Fermi energy in the nodal region, is difficult to verify directly in ARPES experiments, because this effect only appears at positive energy, around $\omega \simeq 100\,\mathrm{meV}$. On the other hand, our more subtle prediction, the combination of superconducting and staggered-flux gaps into a single asymmetric gap, appearing in the anti-nodal region of cuprates may well be within current experimental reach. However, it is clear that any energy symmetrization procedure on experimental data [14] inevitably destroys all such signs in the spectral function.

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