Intertwined orders in the two-dimensional Hubbard model

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Outline

✓ Introduction
✓ Symmetry-entangled mean-field theory and extensions
✓ Intertwined orders
✓ Results and phase diagram
✓ Reliability of the scheme
✓ Further extensions
✓ Summary
The Hubbard model

\[ \hat{H} = -t \sum_{\langle \vec{r}, \vec{r}' \rangle} \hat{c}_{\vec{r}\sigma} \hat{c}_{\vec{r}'\sigma}^{\dagger} + U \sum_{\vec{r}} \hat{n}_{\vec{r}\uparrow} \hat{n}_{\vec{r}\downarrow} \]

Nearest neighbour hopping

On-site interaction

Minimal low energy effective model of electrons in CuO$_2$ planes

Cuprates
The half-filled Hubbard model

\[ \hat{H} = -t \sum_{\langle \vec{r}, \vec{r}' \rangle, \sigma} \hat{c}^{\dagger}_{\vec{r} \sigma} \hat{c}_{\vec{r}' \sigma} + U \sum_{\vec{r}} \hat{n}_{\vec{r} \uparrow} \hat{n}_{\vec{r} \downarrow} \]

Fermionic atoms loaded in optical lattices

Delocalized states

\( U = 0 \)

Mott insulator

One atom per site

\( U >> t \)


Double occupancy

\[ \frac{U}{6t} = 4.8, \ V_0 = 7 \ E_f \]
\[ \frac{U}{6t} = 19, \ V_0 = 12 \ E_f \]
\[ \frac{U}{6t} = 25, \ V_0 = 12 \ E_f \]
The half-filled Hubbard model

\[ \hat{H} = -t \sum_{\langle \vec{r}, \vec{r}' \rangle_\sigma} \hat{c}_{\vec{r} \sigma}^+ \hat{c}_{\vec{r}' \sigma} + U \sum_{\vec{r}} \hat{n}_{\vec{r} \uparrow} \hat{n}_{\vec{r} \downarrow}, \quad U \gg t \]

No tunnelling (Pauli principle)

\[ E_{t=0} = 0 \]

Antiferromagnetic order

\[ \langle \hat{S}_0 \cdot \hat{S}_r \rangle \propto (-1)^{x+y} = \cos(\pi x + \pi y) \]

\[ S(q) = \sum_{\vec{r}} \exp(iq \cdot \vec{r}) \langle \hat{S}_0 \cdot \hat{S}_{\vec{r}} \rangle \text{ peaked at } \vec{q} = (\pi, \pi) \]

R. A. Hart et al., arxiv/cond-mat (2014)
The hole-doped Hubbard model

Antiferromagnetism: \( \langle \hat{S}_r \rangle \propto (-1)^{x+y} \tilde{u}_z \)

Spiral magnetism: \( \langle \hat{S}_r \rangle \propto \cos(\tilde{q}_s \cdot \tilde{r})\tilde{u}_z + \sin(\tilde{q}_s \cdot \tilde{r})\tilde{u}_y \)

Spin density waves: \( \langle \hat{S}_r \rangle \propto \cos(\tilde{q}_s \cdot \tilde{r})\tilde{u}_z \)

and many others ....

Stripes: \( \langle \hat{S}_r \rangle \propto \cos(\tilde{q}_s \cdot \tilde{r})\tilde{u}_z, \langle \hat{n}_r \rangle \propto \cos(\tilde{q}_c \cdot \tilde{r}) \)

d-wave superconductivity: \( \langle \hat{c}_{r} \hat{c}_{r+\tilde{u}_x} \rangle = -\langle \hat{c}_{r} \hat{c}_{r+\tilde{u}_x} \rangle \neq 0 \)
In Fig. 16, it is then possible to create two different quantum states. Because FS is no longer of the shape of a diamond, even for d-SDW order. The left panel shows the evolution of the l-SDW state with doping of 1/32 at $U=1.5$, which gives rise to a SDW with different regions include: l-SDW (SDW state with a linear modulation along [10]), d-SDW (SDW state with a linear modulation along [10]), l-stripes (density determined by fitting our numerical results, and are meant as the l-SDW state) to localized holes is denoted by the state with a long wavelength modulation along the [10]-direction); d-SDW order. The right panel shows the CD and SD along y-axis vs. interacting strengths. The system being studied is a Hubbard model on an infinite lattice with doping of 0.2, 0.4, 0.6, 0.8, 1.0. Each curve is an HF calculation for a different value of U, and the CD and SD are calculated using a mean-field approximation. The figure shows that the CD and SD increase with increasing U, and that the l-SDW state is stabilized at high U. The figure also shows that the CD and SD are independent of the doping level at low U, but become more sensitive to doping at high U.

In this section we present a phenomenological model for the evolution of the UHF ground state in the parameter space of the Hubbard model. The model is based on a variational ansatz for the ground state wave function, which is written as a product of local operators. The variational parameters are determined by fitting the numerical results, and are used to map out the sequence of the evolution of the UHF ground state.

The model is given by

$$\Phi_{HF} = \hat{c}^+_\phi_1 \ldots \hat{c}^+_\phi_N \rangle$$

where $\hat{c}^+_\phi_n$ is the creation operator for a hole at site n with momentum $\phi$. The model is then used to calculate the CD and SD along y-axis vs. interacting strengths, and the results are shown in the figure.


Conventional variational approaches to the Hubbard model

Full N-body Hilbert space
Conventional variational approaches to the Hubbard model

Full N-body Hilbert space

\[ \Phi_{HF} = |\Phi\rangle = |\Phi\rangle_\uparrow |\Phi\rangle_\downarrow \]

\[ \hat{P}^{(Gutz.)} |\Phi_{HF}\rangle \]

Two-body correlator to reduce double occupancy


Conventional variational approaches to the Hubbard model

No mean-field superconductivity

\[ |\Phi_{BCS}\rangle \approx \prod_\alpha \left( u_\alpha + v_\alpha \hat{c}_\alpha^+ \hat{c}_\alpha^\dagger \right) |\rangle \]

\[ \hat{P}^{(Gutz.)} |\Phi_{BCS}\rangle \]

\[ |\Phi_{HF}\rangle = |\Phi\rangle_\uparrow |\Phi\rangle_\downarrow \]

\[ |\Phi_{HF}\rangle = \hat{c}_\phi^+ \cdots \hat{c}_\phi^N \; |\rangle \]

\[ \hat{P}^{(Gutz.)} |\Phi_{HF}\rangle \]

Full N-body Hilbert space

\[ \text{T. Misawa, M. Imada, arxiv/cond-mat (2013)} \]
The symmetry-projected Hartree-Fock/BCS wavefunction

No assumed charge, spin or superconducting orders

Totally unrestricted orthonormal single-particle states
\[
\prod_{i=1}^{N} \hat{c}_{\phi_i}^+ | \phi_i \rangle
\]
with \( \hat{c}_{\phi_i}^+ = \sum_{\tau\sigma} \phi_{i,\tau\sigma} \hat{c}_{\tau\sigma}^+ \)

General unitary Bogoliubov transformation
\[
\propto \prod_{\tilde{r}\tilde{\sigma}} \hat{\gamma}_{\tilde{r}\tilde{\sigma}} | \phi_{\tilde{r}\tilde{\sigma}} \rangle
\]
with \( \hat{\gamma}_{\tilde{r}\tilde{\sigma}} = \sum_{r\sigma'} \left( U_{r\sigma'\tilde{r}\tilde{\sigma}}^* \hat{c}_{r\sigma'}^+ + V_{r\sigma'\tilde{r}\tilde{\sigma}}^* \hat{c}_{r\sigma'}^+ \right) \)

Exact ground state characterized by several quantum numbers \( \Gamma \) reflecting symmetries of the Hamiltonian
\[
\Gamma = (N, \bar{K}, S, S_z, \ldots)
\]

Quantum number projection by superposition of symmetry related wavefunctions
\[
\hat{P}^{(\Gamma)} \propto \sum_{g} \left( \chi_{g}^{(\Gamma)} \right)^* \hat{U}_g
\]

Correlations from restoration of deliberately broken symmetries by projection before variation
\[
\delta E^{(\Gamma)} = \delta \langle H \rangle_{\phi^{(\Gamma)}} = 0
\]
The symmetry-projected Hartree-Fock/BCS wavefunction

The symmetry-projected Hartree-Fock/BCS wavefunction $R_{g}^{a,b}$ is defined as

\[
R_{g}^{a,b} = \begin{pmatrix} \rho_{g}^{a,b} & \kappa_{g}^{a,b} \\ \bar{k}_{g}^{a,b} & \bar{\rho}_{g}^{a,b} \end{pmatrix}
\]

with

\[
\begin{pmatrix} \rho_{g}^{a,b} & \kappa_{g}^{a,b} \\ \bar{k}_{g}^{a,b} & \bar{\rho}_{g}^{a,b} \end{pmatrix} = \frac{1}{N_{g}^{(a,b)}} \left\langle \Phi_{a} \left| \begin{pmatrix} \hat{c}_{\gamma \sigma}^{+} \hat{c}_{\gamma \sigma} & \hat{c}_{\gamma \sigma}^{+} \hat{c}_{\gamma' \sigma} \\ \hat{c}_{\gamma' \sigma}^{+} \hat{c}_{\gamma \sigma} & \hat{c}_{\gamma' \sigma}^{+} \hat{c}_{\gamma' \sigma} \end{pmatrix} \right| \Phi_{b,g} \right\rangle
\]

Generalized eigenvalue problem for the amplitudes

\[
\sum_{b} \left\langle \Phi_{a} \left| \hat{H} \hat{P}^{(\Gamma)} \right| \Phi_{b} \right\rangle c_{b} = E^{(\Gamma)} \sum_{b} \left\langle \Phi_{a} \left| \hat{P}^{(\Gamma)} \right| \Phi_{b} \right\rangle c_{b}
\]

Wick's theorem for matrix elements between mean-field states

One-body transition density matrix

\[
\sum_{g} \left( \chi_{g}^{(\Gamma)} \right)^* N_{g}^{(a,b)} \mathcal{E} \left[ R_{g}^{a,b} \right]
\]

Overlap between HF and/or BCS wave-functions

\[
\sum_{g} \left( \chi_{g}^{(\Gamma)} \right)^* N_{g}^{(a,b)} \text{ with } N_{g}^{(a,b)} = \left\langle \Phi_{a} \left| \Phi_{b,g} \right\rangle \right.
\]
The symmetry-projected Hartree-Fock/BCS wavefunction

Optimal single-particle states and BCS quasiparticles

\[ \Psi(\Gamma_{a,b}) = \left( \begin{array}{c} L(\Gamma_{a,b}) \\ \Lambda(\Gamma_{a,b}) \end{array} \right) = \sum_g \left( \chi_g^{(\Gamma)} \right)^* N_g^{(a,b)} \left[ (1 - R_g^{(a,b)}) \right] \mathcal{H} \left[ R_g^{(a,b)} \right] R_g^{(a,b)} + \frac{1}{\Delta_g} \left( \begin{array}{c} h_g^{(a,b)} \\ \Lambda_g^{(a,b)} \end{array} \right) \right) \]

Bogoliubov-de Gennes Hamiltonian expressed in terms of the one-body transition density-matric

\[ \frac{\partial \mathcal{H}}{\partial \rho_g^{(a,b)}} \bigg|_{\sigma, j', \sigma'} = \frac{\partial \mathcal{E}}{\partial \rho_g^{(a,b)}} \bigg|_{\sigma, j', \sigma'} \]

\[ \frac{\partial \mathcal{H}}{\partial \chi_g^{(a,b)}} \bigg|_{\sigma, j', \sigma'} = \frac{\partial \mathcal{E}}{\partial \chi_g^{(a,b)}} \bigg|_{\sigma, j', \sigma'} \]

\[ \begin{cases} C_{HF} L^{(\Gamma_{HF, BCS})} + C_{BCS} L^{(\Gamma_{HF, BCS})} = 0 \\ C_{HF} \Psi^{(\Gamma_{BCS, BCS})} + C_{BCS} \Psi^{(\Gamma_{BCS, BCS})} = 0 \end{cases} \]

A. Leprévost, O. Juillet and R. Frésard, to be published.
Energy minimization by the conjugate gradient method through Thouless parameterization of HF and BCS wavefunctions

We use a 16x4 supercell with antiperiodic/periodic boundary conditions

$\sim 10^4$ complex variables to be simultaneously determined

Translational invariance and lattice symmetries ($C_{2v}$ group) are restored
+ Particle number projection for the BCS state
+ Spin rotational invariance partially restored during the optimization:
  $S_z$ and spin-parity $\sigma_S = (-1)^S$ projections

The variational N-body state corresponds to the superposition
of $\sim 7.10^4$ symmetry related wavefunctions

Full spin projection after basis optimization

New amplitudes from eigenvalue equation
with totally projected states

Same unprojected basis states
Signatures of spin-density wave and spiral orderings

Classical SDW: \( \vec{S}_y \propto \cos(\vec{q}_s \cdot \vec{r}) \hat{u}_z \)

\[ \phi_r(\vec{r}) = \left\{ \begin{array}{c} \exp(i\vec{q} \cdot \vec{r}) \\ \sum \exp(iq \cdot \vec{r}) \end{array} \right\} \text{ peaked at } \vec{q} = \vec{q}_s \]

\[ \vec{V}_r = \vec{S}_y \wedge (\vec{S}_{r+\hat{u}_x} + \vec{S}_{r+\hat{u}_y}) \]

\[ \propto \cos(\vec{q}_s \cdot \vec{r}) \]

\[ \sin q_{S,x} + \sin q_{S,y} \]

\[ \vec{u}_z = Cte \]

Classical spiral: \( \vec{S}_y \propto \cos(\vec{q}_s \cdot \vec{r}) \hat{u}_z + \sin(\vec{q}_s \cdot \vec{r}) \hat{u}_y \)

\[ 0 \rightarrow \text{ Spin density wave} \]

\[ > 0 \rightarrow \text{ Spiral} \]
Signatures of spin-density wave and spiral orderings

SDW with wavevector $\tilde{q}_S$

Spiral with wavevector $\tilde{q}_S$

$S(\tilde{q}) \propto \delta_{\tilde{q}, \tilde{q}_S}$ and $\mathcal{V}(\tilde{r})_{r \to \infty} = 0$

$S(\tilde{q}) \propto \delta_{\tilde{q}, \tilde{q}_S}$ and $\mathcal{V}(\tilde{r})_{r \to \infty} > 0$

Dependence of magnetic correlations on hole doping at $U=8t$
Signatures of stripe ordering

Related peaks in the Fourier transform of the spin-spin and density-density correlation functions

\[ S(\mathbf{q}) = \sum_{\mathbf{r}} \exp(i\mathbf{q} \cdot \mathbf{r}) \langle \hat{S}_\mathbf{0} \cdot \hat{S}_\mathbf{r} \rangle \]

\[ C(\mathbf{q}) = \sum_{\mathbf{r}} \exp(i\mathbf{q} \cdot \mathbf{r}) \langle \delta \hat{n}_\mathbf{0} \delta \hat{n}_\mathbf{r} \rangle \]

Dependence of magnetic and charge correlations on hole doping

\[ U = 12t \]
Signature of d-wave superconductivity

Long-ranged pair correlations: \( \mathcal{D}(\vec{R}) = \frac{1}{2} \langle \hat{D}^+_0 \hat{D}^-_R + \hat{D}^+_0 \hat{D}^+_{-R} \rangle \xrightarrow{R \to \infty} \text{Cte} \)

Singlet d-wave pair field

\[
\sum_{\vec{r} \in \{ \pm \vec{u}_x, \pm \vec{u}_y \}} f(\vec{r}) \frac{1}{\sqrt{2}} \left( \hat{c}^+_{\vec{R} \uparrow} \hat{c}^+_R - \hat{c}^+_{\vec{R} \downarrow} \hat{c}^+_{R \uparrow} \right) \text{ with } f(\vec{r}) = \begin{cases} +1 & \text{if even } \vec{r} \\ -1 & \text{if odd } \vec{r} \end{cases}
\]

\[
\langle \hat{c}^+_{i \uparrow} \hat{c}^+_{j \downarrow} \hat{c}^+_{k \downarrow} \hat{c}^+_{l \downarrow} \rangle \rightarrow \langle \hat{c}^+_{i \uparrow} \hat{c}^+_{j \uparrow} \hat{c}^+_{k \downarrow} \hat{c}^+_{l \downarrow} \rangle - \langle \hat{c}^+_{i \uparrow} \hat{c}^+_{j \downarrow} \hat{c}^+_{k \downarrow} \hat{c}^+_{l \downarrow} \rangle - \langle \hat{c}^+_{i \uparrow} \hat{c}^+_{j \downarrow} \hat{c}^+_{k \downarrow} \hat{c}^+_{l \downarrow} \rangle \Rightarrow \mathcal{D}(\vec{R}) = 0 \text{ for non-interacting electrons}
\]

Dependence of superconductivity on hole doping

\( U = 12t \)
Phase diagram from symmetry-projected HF/BCS wavefunctions

- **stripe**
  - $\mathbf{q}_c = (\pi/2, 0)$
  - $\mathbf{q}_s = (3\pi/4, \pi/2)$
- **SDW/Spiral**
  - $\mathbf{q}_s = (3\pi/4, \pi)$
  - $\mathbf{q}_s = (3\pi/4, \pi/2)$

Hole doping
- $\mathbf{q}_s = (3\pi/4, \pi)$
- $\mathbf{q}_s = (7\pi/8, \pi)$

U/t
- 12
- 10
- 8
- 6
- 4

U/t
- 12
- 10
- 8
- 6
- 4
Reliability of the symmetry projected HF/BCS scheme

Comparison with exact results at half-filling

$\hat{P}^{(Γ)} |Φ_{HF}\rangle$ is the exact ground-state at any coupling for the 2x2 cluster


<table>
<thead>
<tr>
<th>System</th>
<th>Energy/t</th>
<th>S(π,π)</th>
<th>C(π,π)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4x4 - U = 4t - t' = 0</td>
<td>Ex. Diag.</td>
<td>-13.6224</td>
<td>2.73</td>
</tr>
<tr>
<td></td>
<td>HF – BCS (S = 0)</td>
<td>-13.618</td>
<td>2.743</td>
</tr>
<tr>
<td>6x6 - U = 4t - t' = 0</td>
<td>QMC</td>
<td>-30.87(2)</td>
<td>4.365(3)</td>
</tr>
<tr>
<td></td>
<td>HF – BCS (S = 0)</td>
<td>-30.724</td>
<td>4.562</td>
</tr>
</tbody>
</table>
Reliability of the symmetry projected HF/BCS scheme

Comparison with exact results on doped small clusters

<table>
<thead>
<tr>
<th>4 × 4 − N = 14</th>
<th>U = 8t − t’ = −0.3t</th>
<th>4 × 4 − N = 10 − U = 10t − t’ = 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy/t</td>
<td>$S(\pi, \pi)$</td>
<td>$C(\pi, \pi)$</td>
</tr>
<tr>
<td>$E_{\text{ED}}^{(T)} = -16.902 \ t$</td>
<td>-12.503</td>
<td>0.724</td>
</tr>
<tr>
<td>$\langle \hat{H}\rangle_{\text{HF–BCS } (S=0)} = -16.876 \ t$</td>
<td>0.727</td>
<td>0.279</td>
</tr>
</tbody>
</table>


$E_{\text{ED}}^{(T)} = -10.05 \ t$

$\langle \hat{H}\rangle_{\text{HF–BCS } (S=0)} = -9.957 \ t$
Comparison with the Gutzwiller wavefunction

8x8 lattice - U=10t

\[ \langle \hat{H} \rangle_{HF-BCS}^{(1)} / N \sim \begin{cases} -0.525 \\ -0.536 \quad (S = 0) \end{cases} \]

\[ \langle \hat{H} \rangle_{HF-BCS}^{(2)} / N \sim \begin{cases} -0.826 \\ -0.829 \quad (S = 0) \end{cases} \]

Reliability of the symmetry projected HF/BCS scheme

Comparison with quantum number projection on QMC and Gutzwiller wavefunctions

8x8 lattice - U=4t - N=50 electrons

\[
\langle \hat{H} \rangle_{HF-BCS}^{(\Gamma)} \sim \begin{cases} 
-69.87 \ t \\
-70.13 \ t \ (S = 0) 
\end{cases}
\]

\[
\langle \hat{H} \rangle_{\text{Gutzwiller}}^{(\Gamma)} = -71.4t, \ \langle \hat{H} \rangle_{\text{QMC}}^{(\Gamma)} = -72.5t
\]

T. Misawa, M. Imada, arxiv/cond-mat (2013)
Energy improvements on the symmetry projected HF/BCS scheme

\[ |\Psi_0^{(\Gamma)}\rangle \rightarrow |\Phi_{HF-BCS}^{(\Gamma)}\rangle = \hat{\rho}^{(\Gamma)} \left( \sum_{i=1}^{N_{HF}} c_{HF}^{(i)} |\Phi_{HF}^{(i)}\rangle + \sum_{i=1}^{N_{BCS}} c_{BCS}^{(i)} |\Phi_{BCS}^{(i)}\rangle \right) \]

- Full symmetry restoration during the optimization
- Mixture of unrestricted and restricted HF/BCS wave functions
- States with good quantum number \( S_z \)
- Sequential optimization

16x4 lattice - U=12t - N=56 electrons

| \( N_{HF} \) | \( N_{BCS} \) | Simultaneous optimization | S=0 projection during the energy minimization | \( \frac{\langle \hat{H} \rangle_{HF-BCS}^{(\Gamma)} - E_{HF}^{(\Gamma)}}{|E_{HF}|} \) |
|---|---|---|---|---|
| 1 | 1 | YES | NO | \( \sim -10.48 \% \) |
| 101 | 20 | NO | YES | \( \sim -17.13 \% \) |
| 40 | 0 | NO | YES | \( \sim -14.96 \% \) |

R. Rodríguez-Guzmán, C. Jiménez-Hoyos, G. Scuséria, arxiv/cond_mat (2014)
Energy improvements on the symmetry projected HF/BCS scheme

\[ C(\vec{q}) = \sum_{\vec{r}} \exp(i\vec{q} \cdot \vec{r}) \langle \delta n_{\vec{0}} \delta n_{\vec{r}} \rangle \]

\[ S(\vec{q}) = \sum_{\vec{r}} \exp(i\vec{q} \cdot \vec{r}) \langle \hat{S}_0 \cdot \hat{S}_r \rangle \]

\[ D(\vec{q}) = \sum_{\vec{R}} \exp(i\vec{q} \cdot \vec{R}) \mathcal{O}(\vec{R}) \]

\[ \mathcal{N}_{HF} = 1 \]
\[ \mathcal{N}_{BCS} = 1 \]

\[ \mathcal{N}_{HF} = 101 \]
\[ \mathcal{N}_{BCS} = 20 \]
### The symmetry projected HF/BCS scheme: new or not?

\[
\left| \Psi_0^{(T)} \right\rangle \rightarrow \left| \Phi_{HF}^{(T)} \right\rangle = \hat{P}^{(T)} \left( \sum_{i=1}^{N_{HF}} c_{i}^{\dagger} \left| \Phi_{HF}^{(i)} \right\rangle \right)
\]

\[
\left| \Psi_0^{(T)} \right\rangle \rightarrow \left| \Phi_{BCS}^{(T)} \right\rangle = \hat{P}^{(T)} \left( \sum_{i=1}^{N_{BCS}} c_{i}^{\dagger} \left| \Phi_{BCS}^{(i)} \right\rangle \right)
\]

(*) , (**) : Full symmetry restoration with totally unrestricted wavefunctions

### General features


### Nuclear shell model


### Quantum chemistry


### Hubbard model

#### 1D model

#### 2D model
- R. Rodríguez-Guzmán *et al.*, arxiv/cond-mat (2014)

### Present work
SDW, SDW/Spirals and stripes find their place in the phase diagram of the 2D Hubbard model.

They successively appear for decreasing doping at fixed U and for increasing U at fixed doping.

Coexistence with d-wave superconductivity has been evidenced for long-ranged pairing correlations at strong coupling (U~10t) and up to a hole doping ~0.2, EXCEPT when the holes are totally trapped in stripes.

These features are robust against extensions of the wavefunction.
Intertwined orders in the two-dimensional Hubbard model

Many thanks to Olivier Juillet and Alexandre Leprévost