Topological transitions in mixed-geometry lattices, and dynamics of fermions in one dimension

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Contents

- The FFLO state in 1D-3D crossover (DMFT) (briefly)
- Pairing in *mixed geometries* (mean field)
- Expansion of a band insulator in a lattice (t-DMRG)
- Expansion of an FFLO state (t-DMRG)
- Dynamics of a polaron in 1D (t-DMRG)
The FFLO state in 1D-3D crossover (DMFT) (briefly)

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SUPERCONDUCTIVITY IN OUR LIVES

JR Maglev MLX01 – 581 km/h (Japan, 2003)

fMRI: brain imaging

LHC: Go Higgs!

Future? Superconducting power grid

Long Island, NY
What is superconductivity?

Cooper pairs of spin up and spin down electrons

Not really:  

More like:
The Fermi surface

\[ E_F \propto k_x^2 + k_y^2 \]
High-temperature superconductors: complicated structure, spin plays a role (?) Fermi surfaces (BaKFeAs)

Fe-based superconductors

Cuprates

LaOFeAs

Spin fluctuations


YBCO

Science 328, 441 (2010)
Spin-Population Imbalanced Fermi Gases

1. Magnetism versus Superconductivity

Chandrasekhar-Clogston limit

Chandrasekhar, APL 1962.
Clogston, PRL 1962.

critical magnetic field to break superconductivity

2. Exotic superconducting phase?

Fulde-Ferrell-Larkin-Ovchinnikov States

Oscillating order parameter

\[ \Delta \equiv \Delta_0 \exp(iqx) \quad (\text{FF}) \]
\[ \Delta \equiv \Delta_0 \cos(qx) \quad (\text{LO}) \]

Polarized Superfluid States

fully paired
+ excess unpaired

Sarma, J Phys Chem Solids 1963
Liu & Wilczek, PRL 2003; Sheehy & Radzihovsky, PRL 2006,
Pao, Wu, Yip PRB 2006; Parish et al., PRL 2007,
Pilati & Giorgini PRL 2008, etc.
Spin-imbalanced fermions in 3D elongated traps

Experiments:
- Shin et. al., PRL 97, 030401 (2006)
- Partridge et. al., Science 311, 5760 (2006)
- Partridge et. al., PRL 97, 190407 (2006)
- Nascimbene et. al., PRL 103, 170402 (2009)

QMC:

DMFT:
FFLO in quasi-1D lattices

D. H. Kim, PT, PRB 85, 180508(R) (2012)
Stronger FFLO signature in quasi-1D?

Somewhere between 3D and 1D: an ideal place for FFLO?

The long-range order may stabilize FFLO.

Mean-field theory (T=0)
Parish et al., PRL 99, 250403 (2007)

Experiment in 1D (density profiles)

In 1D, an exact solution gives FFLO, but no long-range order is possible.

In 3D, the FFLO area may be very narrow.
Stronger FFLO signature in quasi-1D?

A bundle of chains: 3D to 1D

Anisotropic 3D optical lattice for DMFT calculations

\[(1D) \ 0 < t \equiv \frac{t_{\perp}}{t_{\parallel}} \leq 1 \ (3D)\]

Homogeneous 2D lattice of trapped 1D chains

\[U \to U_* \ (a \to \infty)\]
Finite temperature phase diagram

(a) $t_1 = 0.2$

(b) $t_1 = 0.4$

(c) $t_1 = 0.8$

(b) FFLO $N_\uparrow$, $N_\downarrow$
(c) cFFLO $N_\uparrow$, $N_\downarrow$
(d) FFLO
(e) FFLO
(f) pSF
(g) FFLO
(h) FFLO
(i) FFLO

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Confirms the mean-field predictions about stability of FFLO in lattices (due to nesting)

**FFLO enhancement in optical lattices**

In contrast, dimensionality does not play a large role, unlike suggested by mean-field: the FFLO is prominent throughout the crossover.

However, a clear dimensionality effect: extremely uniform order parameter in intermediate dimensionality.
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Pairing in *mixed geometries*

- Pairing with spin-imbalance (mass-imbalance)
  - Chandrasekhar-Clogston limit, FFLO, polarized superfluids, breach pair superfluids, etc.
- Pairing in mixed dimensions
  - A couple of theory papers (Tan, Iskin)
- Our question: pairing in *mixed geometries*
- Motivation
  - *Spin-dependent confinement*
  - Spin-dependent lattices experimentally possible (Hamburg, NIST, Dusseldorf, others)
  - Two fermionic atoms (Li, K) trapped, Feshbach resonances (Innsbruck, MIT, others)
  - Novel superfluids? High $T_c$? Polarized superfluid?
Our choice of geometry: honeycomb lattice for the up-component, triangular for the down-component.
Mean-field theory for this system

\[ \mathcal{H} = -t_{\uparrow} \sum_{\langle i,j \rangle} (\hat{a}_{i\uparrow}^{\dagger} \hat{b}_{j\uparrow} + \text{h.c.}) + \epsilon_{\uparrow}^{a} \sum_{i} \hat{n}_{i\uparrow}^{a} + \epsilon_{\uparrow}^{b} \sum_{i} \hat{n}_{i\uparrow}^{b} \]
\[ - t_{\downarrow} \sum_{\langle i,j \rangle} (\hat{a}_{i\downarrow}^{\dagger} \hat{a}_{j\downarrow} + \text{h.c.}) + \epsilon_{\downarrow}^{a} \sum_{i} \hat{n}_{i\downarrow}^{a} \]
\[ \sum_{i,j} (\hat{n}_{i\uparrow}^{a} + \hat{n}_{j\uparrow}^{b}) - \mu \sum_{i} \hat{n}_{i\downarrow}^{a} - U \sum_{i} \hat{n}_{i\uparrow}^{a} \hat{n}_{i\downarrow}^{a} \]

\[ t_{\uparrow} = t_{\downarrow} = 1 \quad U = 5 \]
\[ \epsilon_{\uparrow}^{a} = \frac{\tilde{\epsilon}}{2} \quad \epsilon_{\uparrow}^{b} = -\frac{\tilde{\epsilon}}{2} \quad \epsilon_{\downarrow}^{a} = -3 \]
The non-interacting system: two braches for the honeycomb

\[ \mathcal{H}_0 = \sum_{\vec{k}} \xi_1(\vec{k}) \hat{c}_{1\vec{k}}^\dagger \hat{c}_{1\vec{k}} + \xi_2(\vec{k}) \hat{c}_{2\vec{k}}^\dagger \hat{c}_{2\vec{k}} + \xi_3(\vec{k}) \hat{c}_{3\vec{k}}^\dagger \hat{c}_{3\vec{k}} \]

\[ \hat{c}_{1\vec{k}}^\dagger = u_A \tilde{a}_{\uparrow}(\vec{k}) + u_B \tilde{b}_{\uparrow}(\vec{k}) \]

\[ \hat{c}_{2\vec{k}}^\dagger = v_A \tilde{a}_{\uparrow}(\vec{k}) + v_B \tilde{b}_{\uparrow}(\vec{k}) \]

Fermi-surface match:

\[ \mu_\downarrow = -\mu_\uparrow^2 \]
Interaction at site A

\[ \mathcal{H}_U = -U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

Corresponds to pairing between spin-down and the two honeycomb branches

\[ \mathcal{H}_U = \sum_{\vec{k}} \left[ g_1(\vec{k}) \hat{c}_{1\overrightarrow{k},3,-\overrightarrow{k}}^\dagger \hat{c}_{3,-\overrightarrow{k}}^\dagger + g_2(\vec{k}) \hat{c}_{2\overrightarrow{k},3,-\overrightarrow{k}}^\dagger \hat{c}_{3,-\overrightarrow{k}}^\dagger + h.c. \right] + \frac{|\Delta|^2}{U} \]
Pairing ansatz at site A

$$\Delta = U \langle \hat{a}_{i\downarrow} \hat{a}_{i\uparrow} \rangle$$

 Leads to a momentum-dependent coupling in the momentum space

$$g_{1,2}(\vec{k}) = -\frac{\Delta}{\sqrt{2}} \left[ 1 \pm \frac{\bar{\epsilon}}{\sqrt{\bar{\epsilon}^2 + |h_{\uparrow}(\vec{k})|^2}} \right]^{\frac{1}{2}}$$

$$h_{\uparrow}(\vec{k}) = -t_{\uparrow} \left[ e^{\frac{ik_x}{\sqrt{3}}} + 2e^{\frac{-ik_x}{2\sqrt{3}}} \cos \frac{k_y}{2} \right]$$
Diagonalize by a Bogoliubov transformation (third order eigenvalue equation)

\[ \mathcal{H} = \sum_{\vec{k}} E_1(\vec{k}) \tilde{\gamma}^\dagger_{1\vec{k}} \tilde{\gamma}_{1\vec{k}} + E_2(\vec{k}) \tilde{\gamma}^\dagger_{2\vec{k}} \tilde{\gamma}_{2\vec{k}} + E_3(\vec{k}) \tilde{\gamma}^\dagger_{3\vec{k}} \tilde{\gamma}_{3\vec{k}} + \sum_{\vec{k}} \xi_{\downarrow}(-\vec{k}) + \frac{|\Delta^2|}{U} \]

\[
\begin{pmatrix}
\tilde{\gamma}_{1\vec{k}} \\
\tilde{\gamma}_{2\vec{k}} \\
\tilde{\gamma}_{3\vec{k}}
\end{pmatrix}
= \mathbf{U}_\vec{k}^\dagger
\begin{pmatrix}
\hat{c}_{1\vec{k}} \\
\hat{c}_{2\vec{k}} \\
\hat{c}_{3,-\vec{k}}^\dagger
\end{pmatrix}
\]
Find the phases by minimizing the grand potential, and from the gap equation

\[ \Omega = - \frac{1}{\beta} \sum_{\vec{k}} \left[ \ln \left( 1 + e^{-\beta E_1(\vec{k})} \right) + \ln \left( 1 + e^{-\beta E_2(\vec{k})} \right) + \ln \left( 1 + e^{-\beta E_3(\vec{k})} \right) \right] + \sum_{\vec{k}} \xi_{\downarrow}(\vec{k}) + \frac{|\Delta|^2}{U} \]
The Fermi surface
Results
Three quasiparticle branches

\[ \mu_\uparrow = -0.1, \ \mu_\downarrow = -1.505, \ U = 5, \ \Delta = 0.93 \]
The phase diagram

\[ P = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}} \]

- **Normal**
- **Forbidden**
- **Gapless iBP**
- **2-FS-(\(\Gamma, K\))**
- **1-FS-(\(\Gamma\))**
- **2-FS-(K,K)**
- **1-FS-(K)**
- **Fully occupied down-spin band**

up-spin density (majority)

Polarization
A new stable polarized superfluid phase: \textit{incomplete breach pair (iBP) state}

Quantum phase transitions between topologically distinct states
Changing the energy offset between the A and B sites
Multiband pairing

energy dispersion $(K-\Gamma)$

noninteracting

interacting

$\xi^\uparrow(k)$

$-\xi^\downarrow(-k)$

$E=0$

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Motivation

- Dynamics of a many-body Fermion system

Core expansion speed as a function of interaction
The system

\[ H = U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - J \sum_{i, \sigma = \uparrow, \downarrow} c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + h.c. \]

J. Kajala, F. Massel, PT, PRL 106, 206401 (2011)

Earlier 1D dynamics: Kollath, Schollwöck, Zwerger, Heidrich-Meisner, Rigol, Cirac, Zoller, Shlyapnikov, Daley, Santos, Carr, Pupillo, Tezuka, Ueda, Diehl, our group, etc.
Results (t-DMRG)

\[ \sqrt{n_{\uparrow}} \text{ for } \frac{|U|}{J} = 0.0 \]
$\sqrt{n_\uparrow}$ for $\frac{|U|}{J} = 1.0$
\[ \sqrt{n_\uparrow} \quad \text{for} \quad \frac{|U|}{J} = 10.0 \]
• With TEBD one can also calculate the doublon density

\[ n_i^{\uparrow \downarrow}(t) = \langle \Phi(t) | c_i^{\dagger \uparrow} c_i^{\dagger \downarrow} c_i^{\downarrow \uparrow} c_i^{\downarrow \downarrow} | \Phi(t) \rangle \]

• Here we call doublons excitations of the form \( c_i^{\dagger \uparrow} c_i^{\dagger \downarrow} | \emptyset \rangle \)
Left: $\sqrt{n_\uparrow}$, Right: $\sqrt{n_{\uparrow\downarrow}}$, $\frac{|U|}{J} = 10.0$
Experiment by Schneider et al., 2D

Our simulation, 1D
• Our explanation for the numerical findings: describe the two last sites by the Hubbard dimer
• We are interested in the paired state $\leftrightarrow$ singlet time evolution.
• The singlet state $\frac{1}{\sqrt{2}}(|\uparrow, \downarrow > - |\downarrow, \uparrow >)$
• $n_{\text{Singlet}}(t) = \frac{8}{16 + \frac{U^2}{J^2}} \left( 1 - \cos \left( \sqrt{U^2 + 16J^2t} \right) \right)$
• Compare to numerics
\[ \sqrt{n_{\text{Singlet}}(t)} \text{ for } \frac{|U|}{J} = 5.0 \]
The frequency comparison.

- TEBD frequency
- Two-site model frequency

Angular frequency (J)

Interaction $|U|$ (J)
The amplitude comparison.

\[ \tilde{n}_\uparrow, \tilde{n}_\downarrow \text{ 1st Osc. amplitude} \]

Interaction \(|U| \text{ (J)}\)

- TEBD
- Two-site model
The amplitude decay comparison.
In the light of the Dimer analysis, let us take another look at the TEBD results.
\[ \sqrt{n_\uparrow} \text{ for } \frac{|U|}{J} = 10.0 \]

\[ n_{\text{Singlet}}(t) = \frac{8}{16 + \frac{U^2}{J^2}} \left( 1 - \cos \left( \sqrt{U^2 + 16J^2t} \right) \right) \]
\[ \sqrt{n_{\uparrow}(1)} \text{ for } \frac{|U|}{J} = 1.0 \]

\[ n_{\text{Singlet}}(t) = \frac{8}{16 + \frac{U^2}{J^2}} \left( 1 - \cos \left( \sqrt{U^2 + 16J^2t} \right) \right) \]
Experiment by Schneider et al., 2D

Our simulation, 1D
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Expansion of an FFLO state in a 1D lattice

Inspired by the (continuum) 1D experiment: Liao et al., Nature 467, 567 (2010)

J. Kajala, F. Massel, PT, PRA 106, 206401(R) (2011)
FFLO in 1D lattice

The doublon density as a function of time $n_{\uparrow\downarrow}(t)$. Interaction $\frac{|u|}{J} = 10.0$. 
The unpaired particle density as a function of time $n_\uparrow(t) - n_{\uparrow\downarrow}(t)$. Interaction $\frac{|V|}{J} = 10.0$. 
$v_{un}^{max} = 2J \sin(k_{un}^{max})$
$v_{\uparrow\downarrow}^{max} = 2J \sin(k_{\uparrow\downarrow}^{max})$

We find that $k_{\uparrow\downarrow}^{max} = k_{\downarrow}$
and $k_{un}^{max} = q$.

Therefore, by measuring the maximum expansion velocity of the unpaired particles, one can detect the \textit{FFLO} momentum. The wavefront corresponding to the maximum velocity is the cloud edge.

$q = \arcsin\left(\frac{V_{\text{max}}}{2J}\right)$. 

Consistent with Bethe ansatz in the large U limit
In trap, + comparison with an uncorrelated (non-FFLO) state
Summary: measuring the expansion velocity of the edge (majority particles) gives the FFLO q-vector!

J. Kajala, F. Massel, PT, PRA 106, 206401(R) (2011)

c.f. C.J. Bolech, F. Heidrich-Meisner, S. Langer, I.P. McCulloch, G. Orso, M. Rigol, PRL 109, 110602 (2012): FFLO correlations lost during the expansion; however, as we point out the initial FFLO q is imprinted to the fastest majority particles that travel at the edge of the cloud.
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- **Dynamics of a polaron in 1D** (t-DMRG)
Dynamics of an impurity in a one-dimensional lattice


Polarons in 2D/3D
Grimm, Zwierlein, Köhl, Salomon, Zwerger, Chevy, Lobo, Bruun etc.

c.f. 1D impurity dynamics experiments for bosons:
Inguscio group, Bloch group
Kick to the down particle: $k = 0.1 \pi$

$$H = -J \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i+1,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_i n_{i,\downarrow} \left(i - \frac{L-1}{2}\right)$$

Bath of up-fermions, one down-particle, lattice for both, trap only for the impurity. Kick of $k$ to the impurity: oscillations observed (t-DMRG)
Doublon dynamics: strong interactions $\langle n_i^{\uparrow}n_i^{\downarrow}\rangle(t)$

$N_\uparrow = 20$

$N_\uparrow = 60$

$N_\uparrow = 140$

$N_\uparrow = 180$

$N_\uparrow = 100$ half filling
Doublon dynamics: weak interactions $\langle n_i \uparrow n_i \downarrow \rangle(t)$

$N_\uparrow = 20$

$N_\uparrow = 60$

$N_\uparrow = 140$

$N_\uparrow = 180$

$N_\uparrow = 100$ half filling
Fourier transform (doublon center of mass motion) 
**strong interactions U/J=10**

**Below half-filling**

**Above half-filling**
Bound on-site pair dynamics (derived from Bethe ansatz)

\[ m_{\text{double}} = \left[ \left( \frac{\partial^2 E}{\partial \kappa^2} \right) \right]^{-1}_{\kappa \to 0} = \frac{1}{J} \sqrt{1 + \frac{U^2}{16J^2}} \frac{|U|/J \gg 1}{4J^2} \]

\[ \Delta E = \omega_{hi} + 2J \left[ (1 - \cos k_p) - (1 - \cos k_F \uparrow) \right] \]

Dynamics of free impurity + impurity mediated bath scattering

Independent of U!
Bound on-site pair dynamics (derived from Bethe ansatz)

\[ m_{\text{double}} = \left[ \left( \frac{\partial^2 E}{\partial \kappa^2} \right) \right]^{-1} \approx \frac{1}{J} \sqrt{1 + \frac{U^2}{16J^2}} \quad \text{as} \quad |U|/J \gg 1 \implies \frac{|U|}{4J^2} \]
Offset: non-uniform $k_F^\uparrow(x)$ due to Friedel oscillations

\[ \Delta E = \omega_{hi} + 2J \left[ (1 - \cos k_p) - (1 - \cos k_F^\uparrow) \right] \]
Fourier transform (doublon center of mass motion), weak interactions $U/J=1$
Polaron peak:

\[ \omega_{\text{pol}} = E_\uparrow + E_\downarrow - E_{\uparrow\downarrow} = -2J \left[ 1 + \cos(k_F\uparrow) \right] + \sqrt{U^2 + 16J^2} \]

\[ |\Psi\rangle = \sqrt{Z}c_{0\downarrow}^\dagger|FS\rangle_\uparrow|0\rangle_\downarrow + \sum_{k > k_F, q < k_F^\dagger} \phi_{k,q} c_{k\uparrow}^\dagger c_{q\uparrow}^\dagger c_{q-k\downarrow}^\dagger |FS\rangle_\uparrow|0\rangle_\downarrow \]
**Summary**

Virtual pair breaking; Polaron internal dynamics

| $|U|$ range | Bath population      | Dynamics regime             |
|------------|----------------------|-----------------------------|
| Strong interaction | Large $N_\uparrow$    | Free particle               |
| Strong interaction | Intermediate $N_\uparrow$ | Bound pair + polaron internal dynamics |
| Strong interaction | Small $N_\uparrow$     | Bound pair                  |
| Weak interaction   | Large $N_\uparrow$     | Free particle               |
| Weak interaction   | Intermediate & small $N_\uparrow$ | Free particle + polaron     |

Same phenomena seen also for strongly repulsive bosonic bath, in the weak interaction case

Pair –free particle scattering; Pair breaking

$$\omega_{pol} = E_\uparrow + E_\downarrow - E_\uparrow\downarrow = -2J [1 + \cos(k_F \uparrow)] + \sqrt{U^2 + 16J^2}$$

$$|\Psi\rangle = \sqrt{Z} c_{0\downarrow}^+ |FS\rangle_\uparrow |0\rangle_\downarrow + \phi_{k_F \uparrow} c_{k_F \uparrow}^+ c_{0\uparrow}^+ c_{0\downarrow}^+ |FS\rangle_\uparrow |0\rangle_\downarrow$$

Virtual pair breaking; Polaron internal dynamics

$$|\Psi\rangle = \sqrt{Z} |FS - 1\rangle_\uparrow |Pair\rangle_\uparrow\downarrow + \phi_{\pi, k_F \uparrow} c_{\pi \uparrow}^+ c_{k_F \uparrow}^+ |FS - 1\rangle_\uparrow |Pair\rangle_\uparrow\downarrow$$
Conclusions

- The FFLO state in 1D-3D crossover (DMFT) (briefly)
  - Intermediate dimension and polarization stabilizes FFLO
- Pairing in *mixed geometries* (mean field)
  - New iBP state, topological transitions, stability of exotic superfluidity connected with multiband pairing
- Expansion of a band insulator in a lattice (t-DMRG)
  - Two-site Hubbard physics describes the dynamics well
- Expansion of an FFLO state (t-DMRG)
  - FFLO directly visible in the free particle expansion
- Dynamics of a polaron in 1D (t-DMRG)
  - Bound pair and new types of polaron dynamics
Dong-Hee Kim (1.3.2013 assistant professor at GIST, South Korea)

Joel Lehikoinen
(now at his own start-up)

Miikka Heikkinen

Francesco Massel
(now at University of Helsinki)

Jussi Kajala
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