d-wave superconducting phase diagram of the two dimensional Hubbard model

A.-M. Tremblay

Giovanni Sordi, Patrick Sémon

Y47.00001 8:00 AM–8:12 AM, Friday March 7, 2014
APS March meeting, Denver, Colorado
Strongly correlated vs weakly correlated: AFM as an example

\[ n = 1, \text{ unfrustrated } d = 3 \text{ cubic lattice} \]

\[ J = \frac{4t^2}{U} \]

Diagram showing the transition between Slater, Heisenberg, and AFM phases as a function of temperature (T) and interaction parameter (U). The Mott transition is also indicated.
Strongly correlated vs weakly correlated: AFM as an example

$n = 1, d = 2$ square lattice

Understanding finite temperature phase from a mean-field theory down to $T = 0$

Critical point visible in $V_2O_3,$ $BEDT$ organics
A finite-doping first order transition, linked to Mott transition up to optimal doping

Doping dependence of critical point as a function of $U$

Sordi et al. PRL 2010, PRB 2011
Model and Method
Hubbard model

\[ H = - \sum_{<ij>\sigma} t_{i,j} \left( c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]
$h$-doped cuprates are strongly correlated
C-DMFT

Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

\[
Z = \int D[\psi^+, \psi] e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_k \psi_k^\dagger(\tau) \Delta(\tau, \tau') \psi_k(\tau')} 
\]

Effective local impurity problem

Effective bath
\[ G_0(i\omega_n) \]

THE DMFT LOOP
\[ G(i\omega_n) \]

Self-consistency condition

\[
\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) 
- \left[ \sum_k \frac{1}{i\omega_n + \mu - t_c(\vec{k}) - \Sigma_c(i\omega_n)} \right]^{-1} 
\]
Standard 2 operator updates in CTQMC are not ergodic in SC state (fixed here)

Please ask in question period…
4 vs 2 operator updates: d-wave order parameter

$U/t = 9$
$T/t = /100$

P. Sémon, G. Sordi, A.-M.S. Tremblay, arxiv.org/1402.7087
Compare ED solver: Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST
Superconductivity at $U > U_{MIT}$
Dome moves to larger dopings with $U$

Max. at lowest $T$ follows N.S. first order transition
c-axis Superfluid density $U = 9t$, $T=1/100$

See also, Gull Millis, PRB, 2013

Panagopoulos et al. PRB 2000
Compare with number of carriers

Peets et al. PRL 2009, Phillips and Jarrell, PRL 2010
Phase diagram for $U = 6.2 \, t$

P. Sémon, G. Sordi, A.-M.S. Tremblay, arxiv.org/1402.7087
$T_c^d$
Meaning of $T_c^d$

- Local pair formation

However, our measurements demonstrate that the nodal gap does not change with reduced doping. The pairing strength does not get weaker or stronger as the Mott insulator is approached; rather, it saturates.

Summary

- CTQMC hybridization expansion needs 4 operator updates on plaquette with d-wave SC
- Strongly correlated superconductivity
  - \( T=0 \) max OP scales with 1st order transition
  - Superfluid density scales like doping beyond max. \( T_c^d \) and beyond max. OP.
  - \( T_c^d \) does not scale with \( T=0 \) d-wave order-parameter in underdoped regime.
André-Marie Tremblay

Sponsors:
Mammouth
Merci
Thank you
Ergodicity of the hybridization expansion with two operator updates and broken symmetry

\[ H_{\text{imp}} = H_{\text{loc}}(d_i^\dagger, d_i) + \sum_{i\mu}(V_{\mu i}a_{\mu}^\dagger d_i + V_{\mu i}^*d_i^\dagger a_{\mu}) \]

\[ + \sum_{\mu} \epsilon_{\mu} a_{\mu}^\dagger a_{\mu}, \]

\[ Z = \text{Tr} \text{T}_{\tau} e^{-\beta H_0} e^{-\int_0^\beta d\tau (H_{\text{hyb}}(\tau) + H_{\text{hyb}}^\dagger(\tau))} \]

\[ = \sum_{k \geq 0} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau_1' \cdots d\tau_k' \text{Tr} \text{T}_{\tau} e^{-\beta H_0} \]

\[ \times H_{\text{hyb}}(\tau_1) H_{\text{hyb}}^\dagger(\tau_1') \cdots H_{\text{hyb}}(\tau_k) H_{\text{hyb}}^\dagger(\tau_k'). \]

\[ \text{Tr}[d_{\uparrow}(0, \pi) d_{\downarrow}(0, \pi) d_{\downarrow}^\dagger(\pi, 0) d_{\uparrow}^\dagger(\pi, 0)] \]

\[ \times F_{\uparrow}(0, \pi), \downarrow(0, \pi) \overline{F}_{\uparrow}(\pi, 0), \downarrow(\pi, 0) \]

P. Sémon, G. Sordi, A.-M.S. Tremblay, arxiv.org/1402.7087