

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



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Y47.00001 8:00 AM–8:12 AM, Friday March 7, 2014

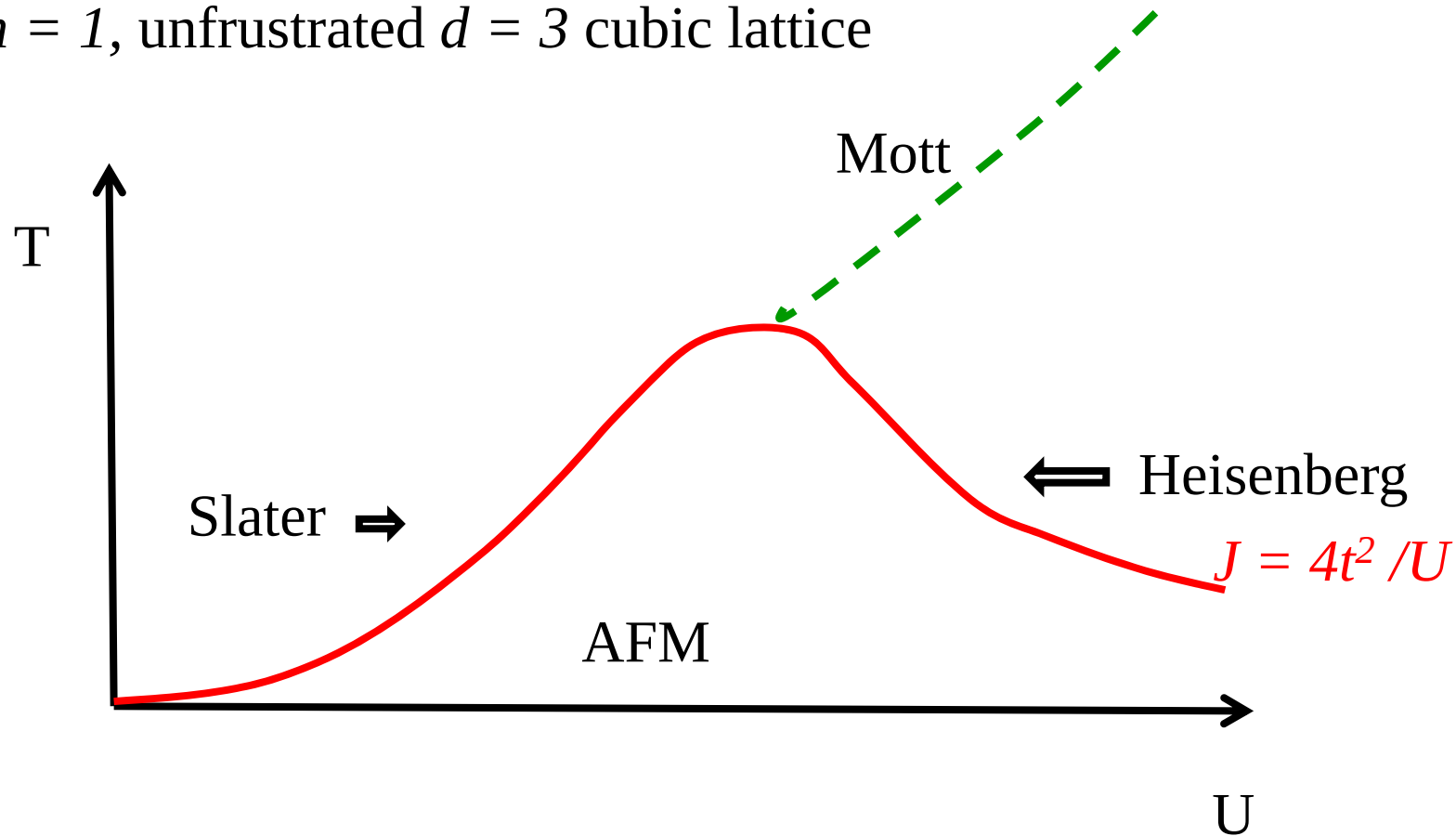
APS March meeting, Denver, Colorado



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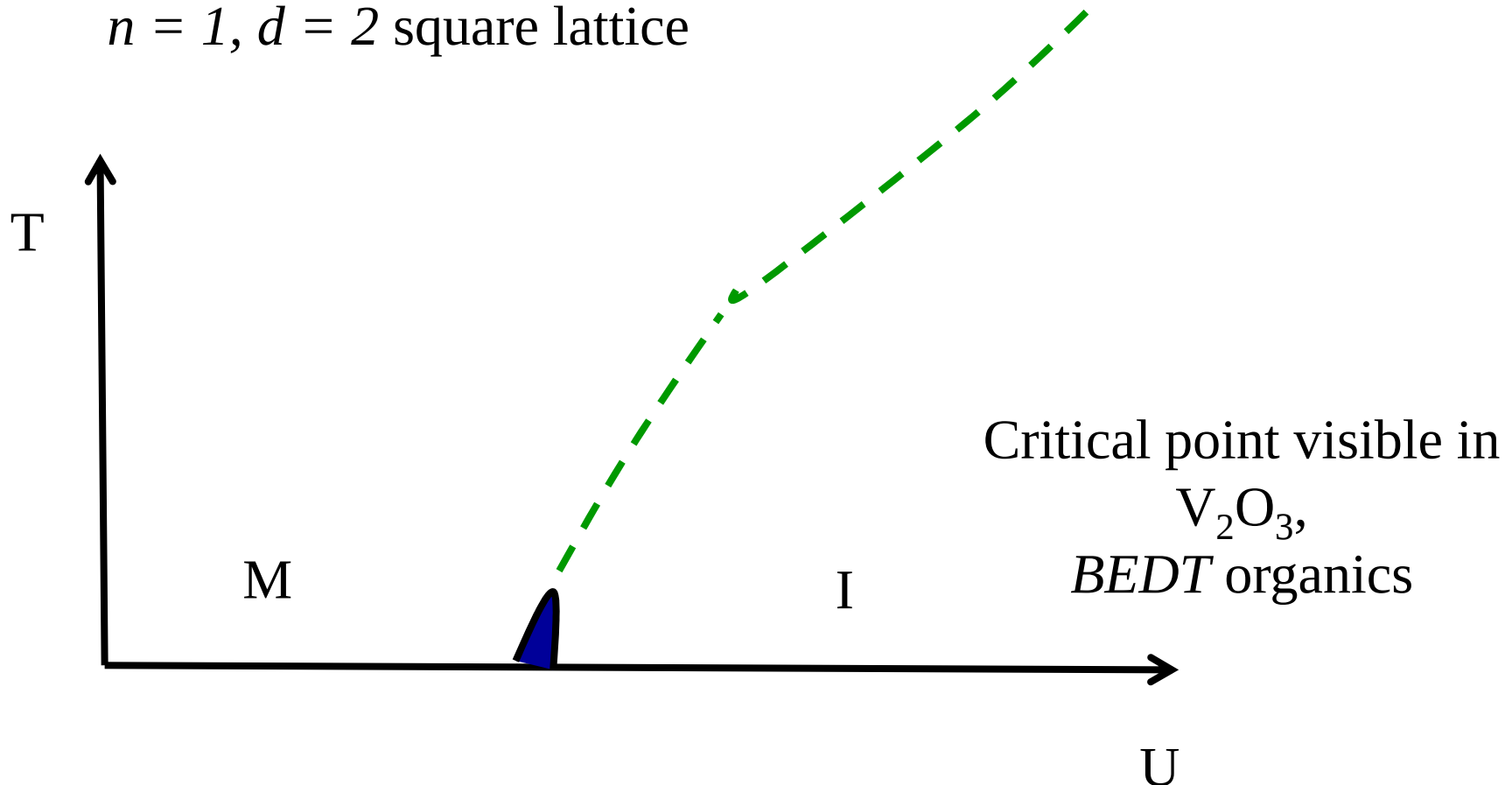
Strongly correlated vs weakly correlated: AFM as an example

$n = 1$, unfrustrated $d = 3$ cubic lattice



Strongly correlated vs weakly correlated: AFM as an example

$n = 1, d = 2$ square lattice

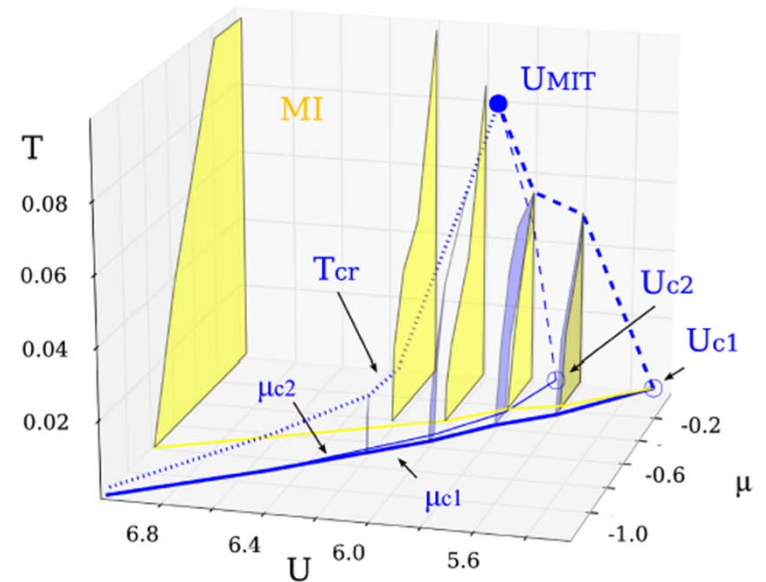
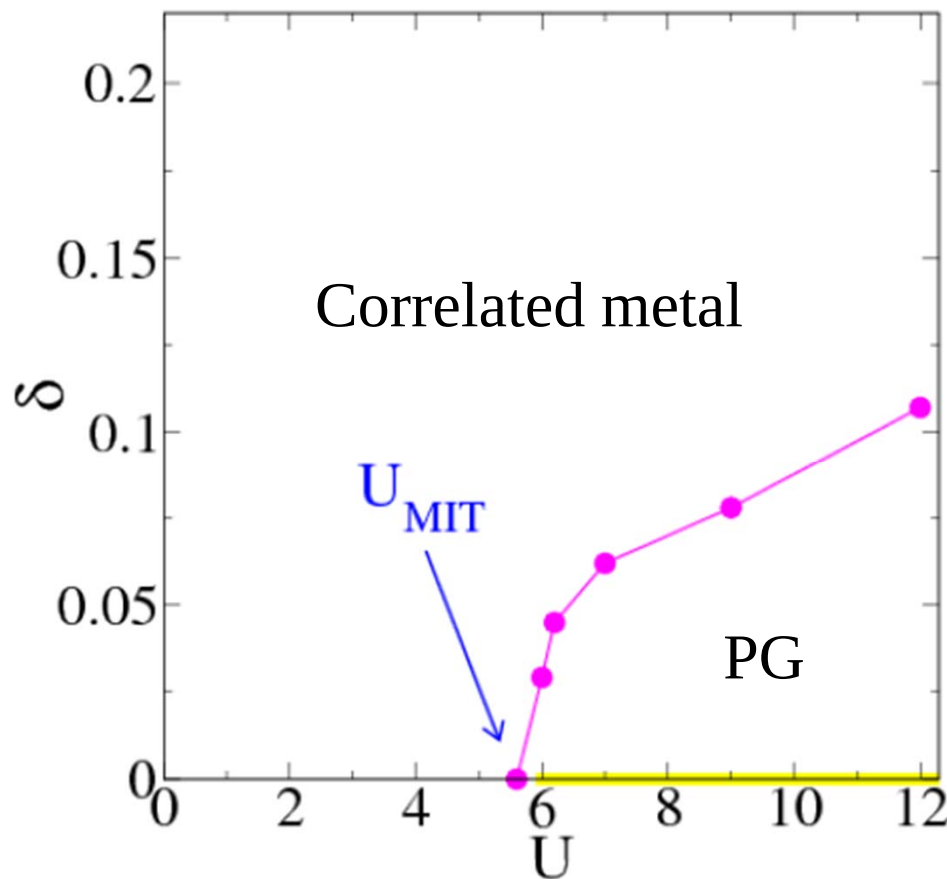


Understanding finite temperature phase from a *mean-field theory* down
to $T = 0$



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



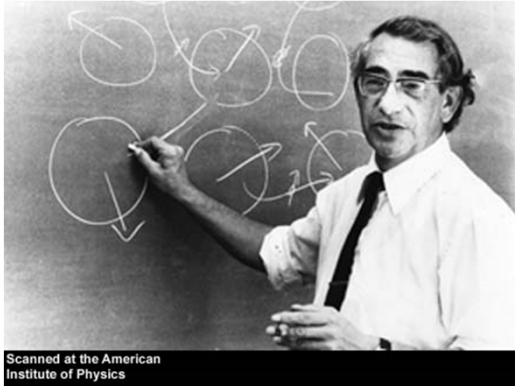
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Model and Method

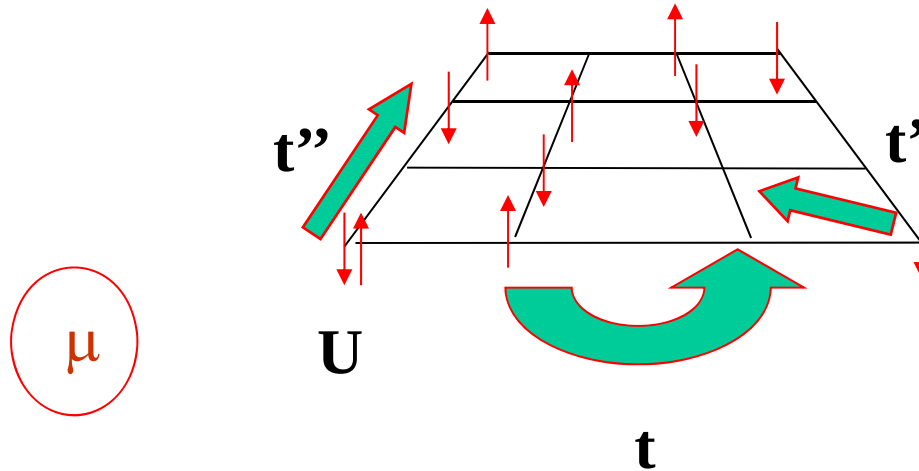


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Hubbard model

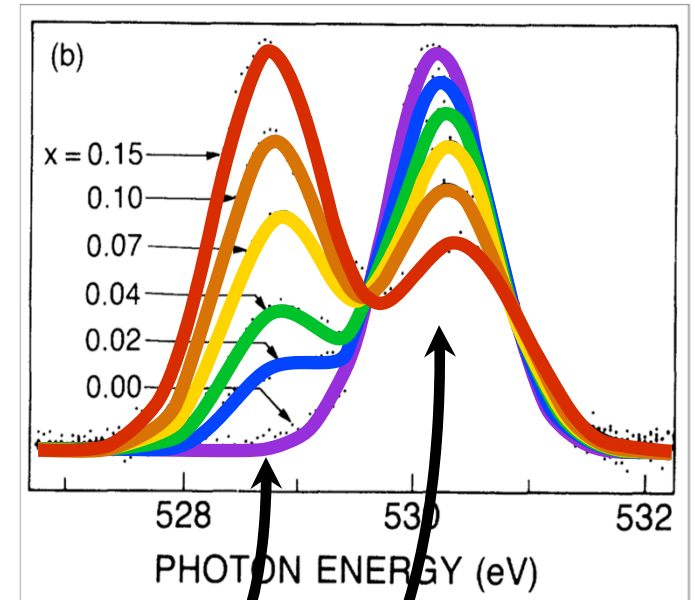
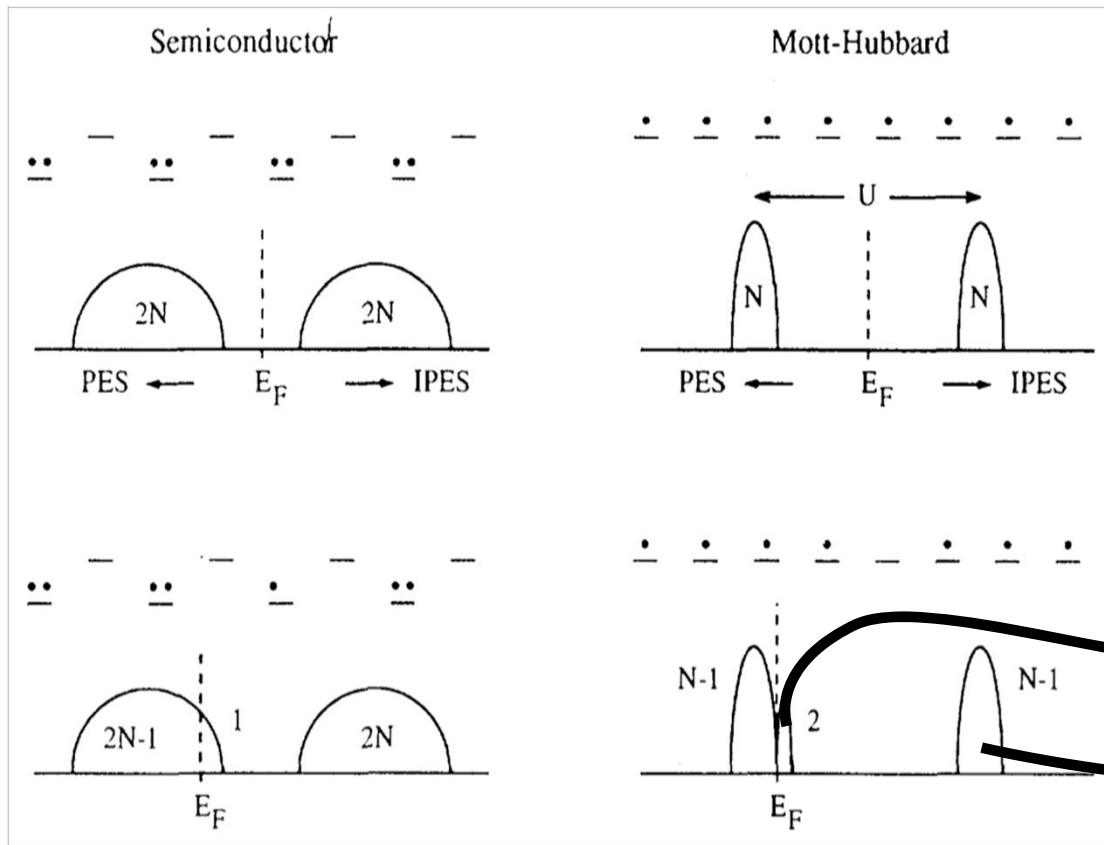


1931-1980

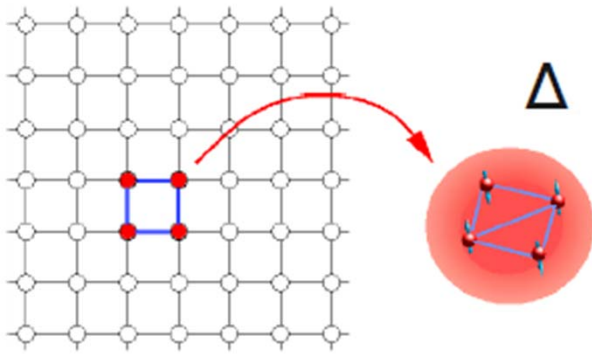


$$H = -\sum_{\langle ij \rangle \sigma} t_{i,j} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

h-doped cuprates are strongly correlated



C-DMFT

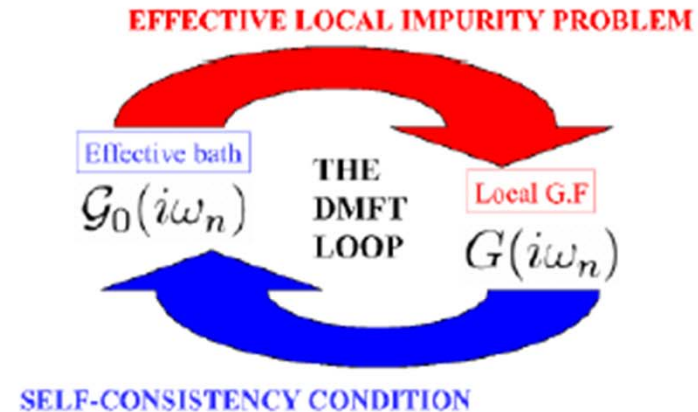


Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

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

$$Z = \int \mathcal{D}[\psi^\dagger, \psi] e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger(\tau) \Delta_{\mathbf{k}}(\tau, \tau') \psi_{\mathbf{k}}(\tau')}$$



$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n)$$

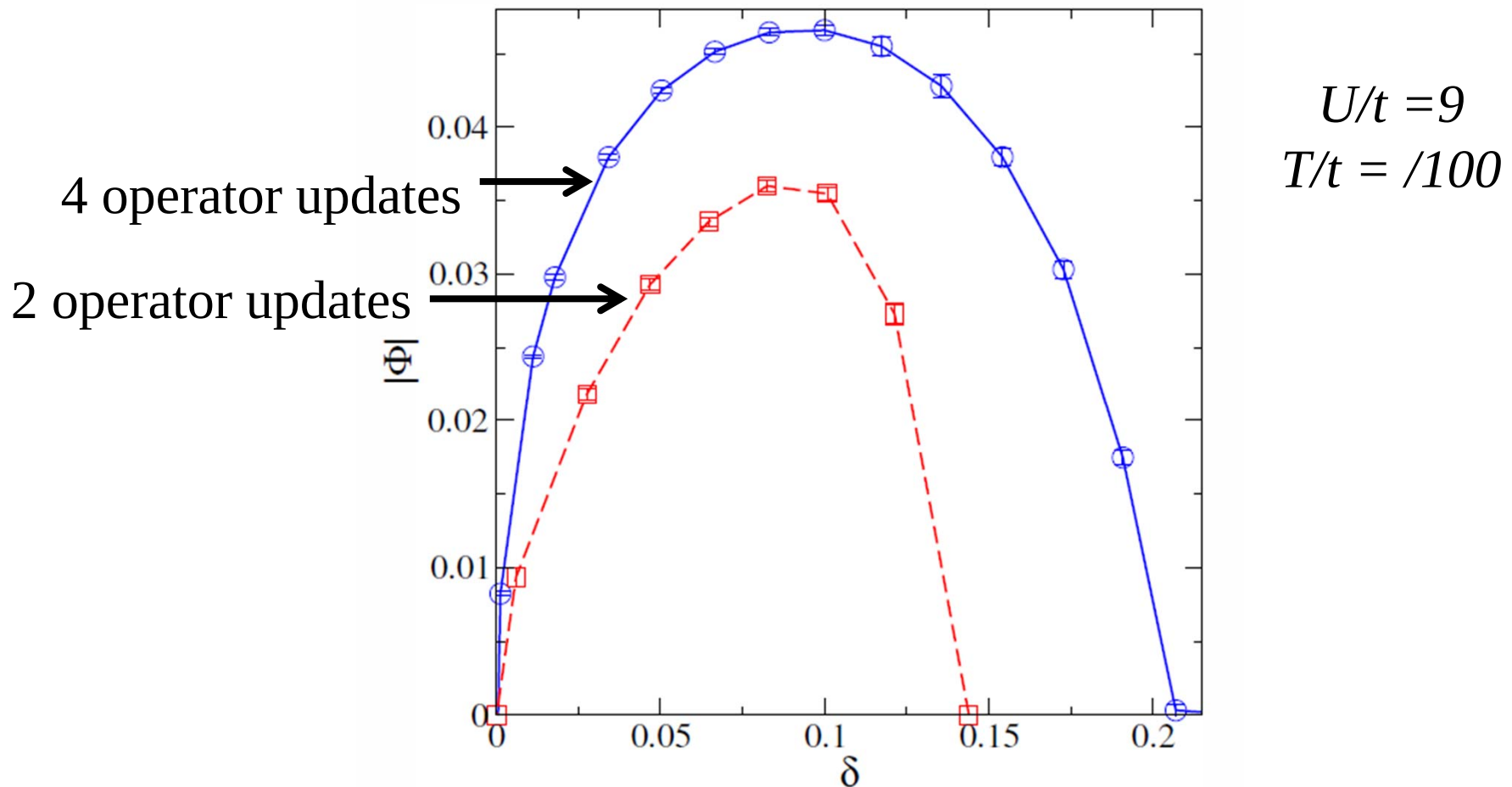
$$- \left[\sum_{\tilde{\mathbf{k}}} \frac{1}{i\omega_n + \mu - t_c(\tilde{\mathbf{k}}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

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



P. Sémon, G. Sordi, A.-M.S. Tremblay, [arxiv.org/1402.7087](https://arxiv.org/abs/1402.7087)

Compare ED solver: Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST

Phys. Rev. B (2008)



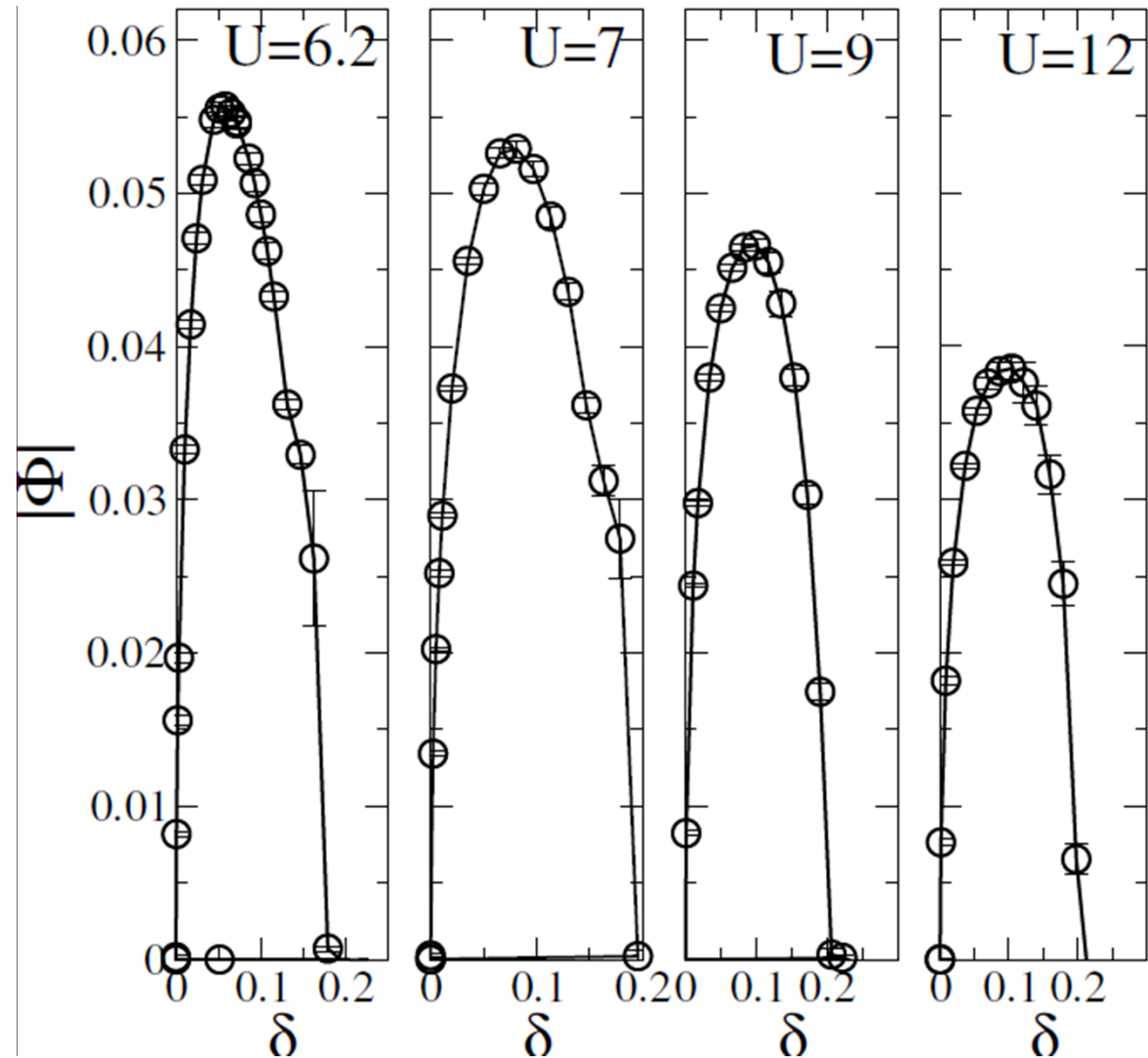
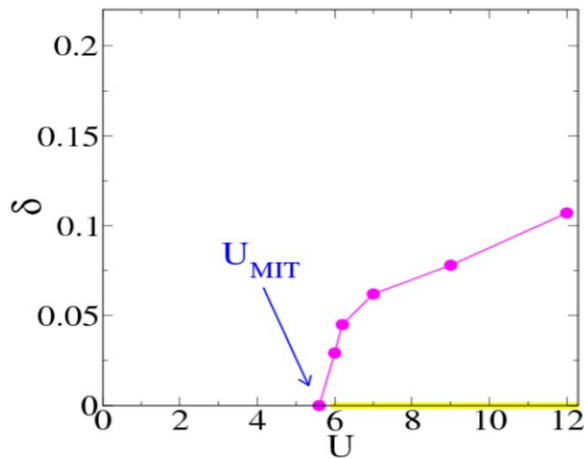
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Superconductivity at $U > U_{MIT}$



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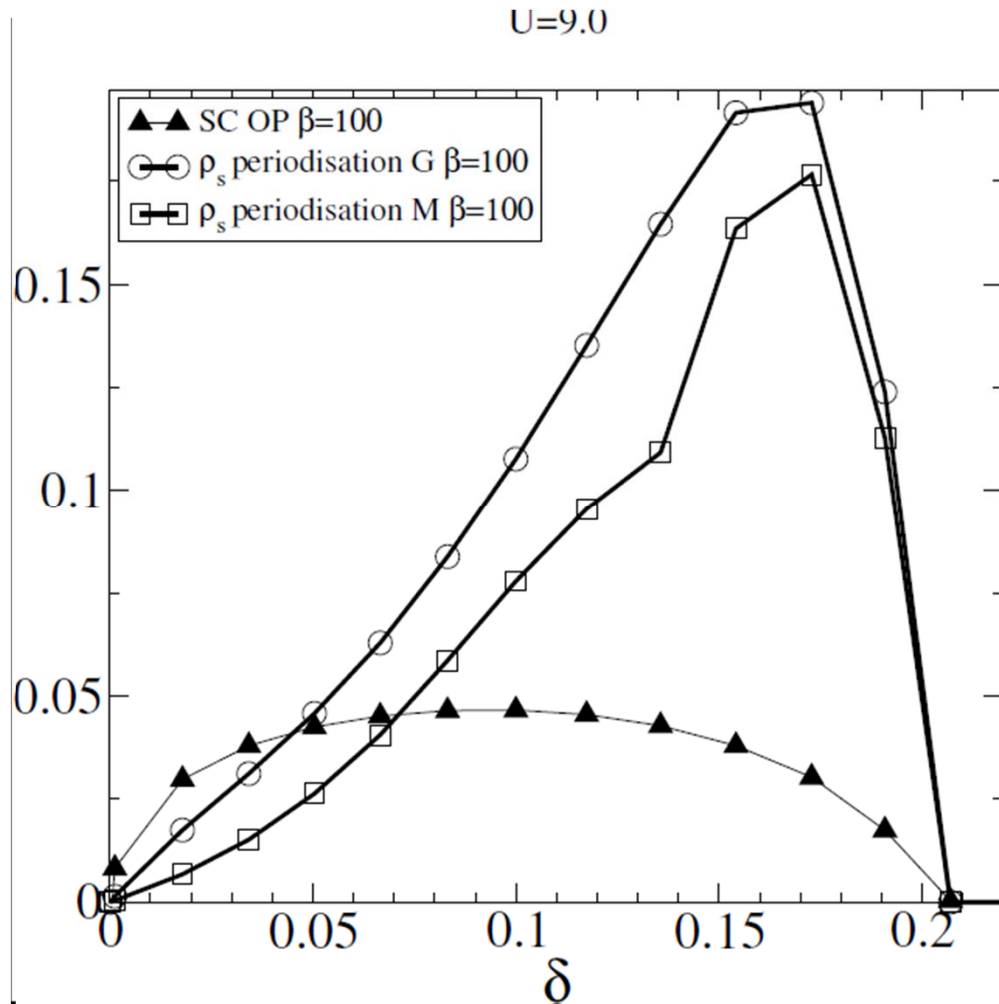
Dome moves to larger dopings with U



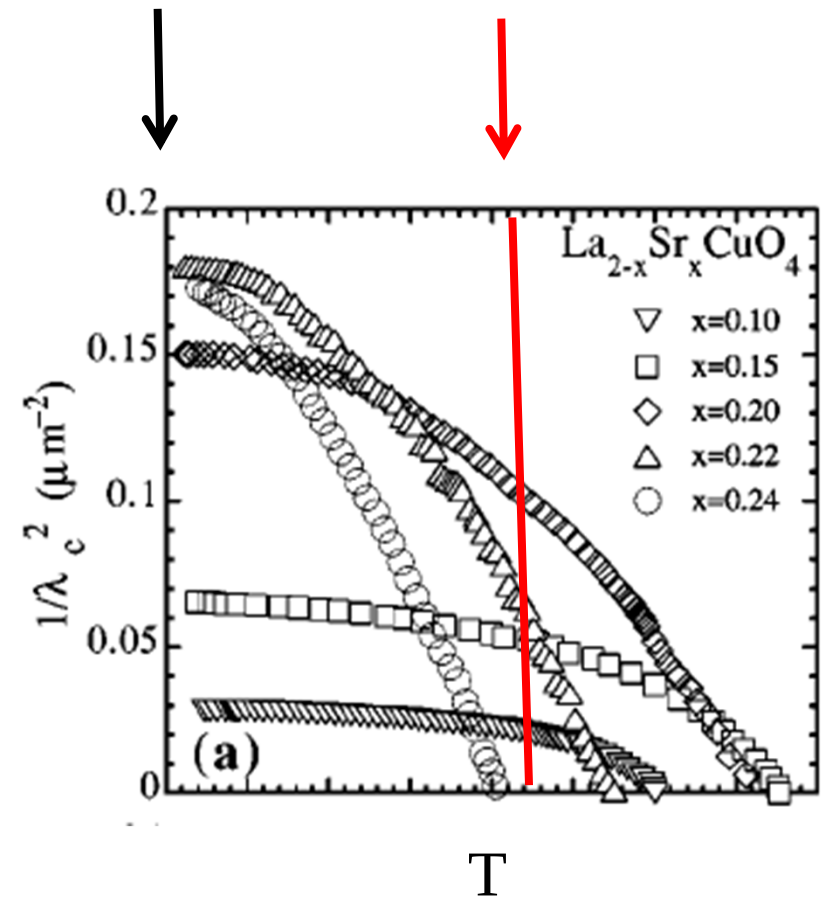
Max. at lowest T follows N.S. first order transition



c-axis Superfluid density $U = 9t, T=1/100$

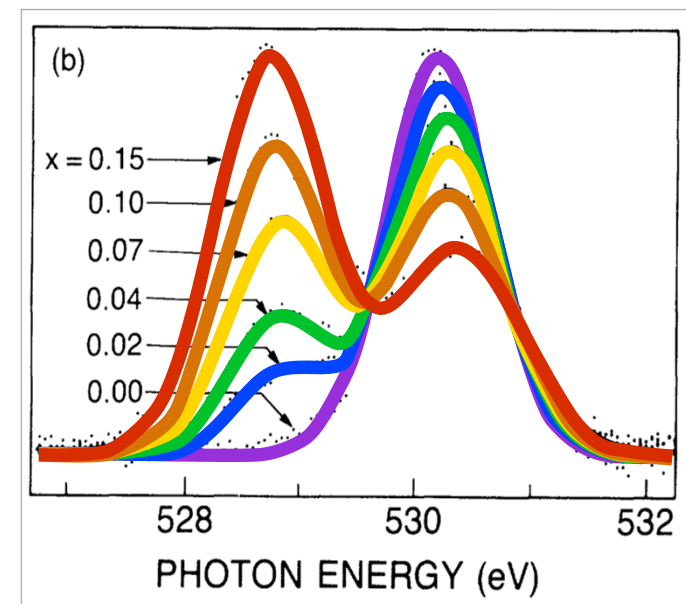
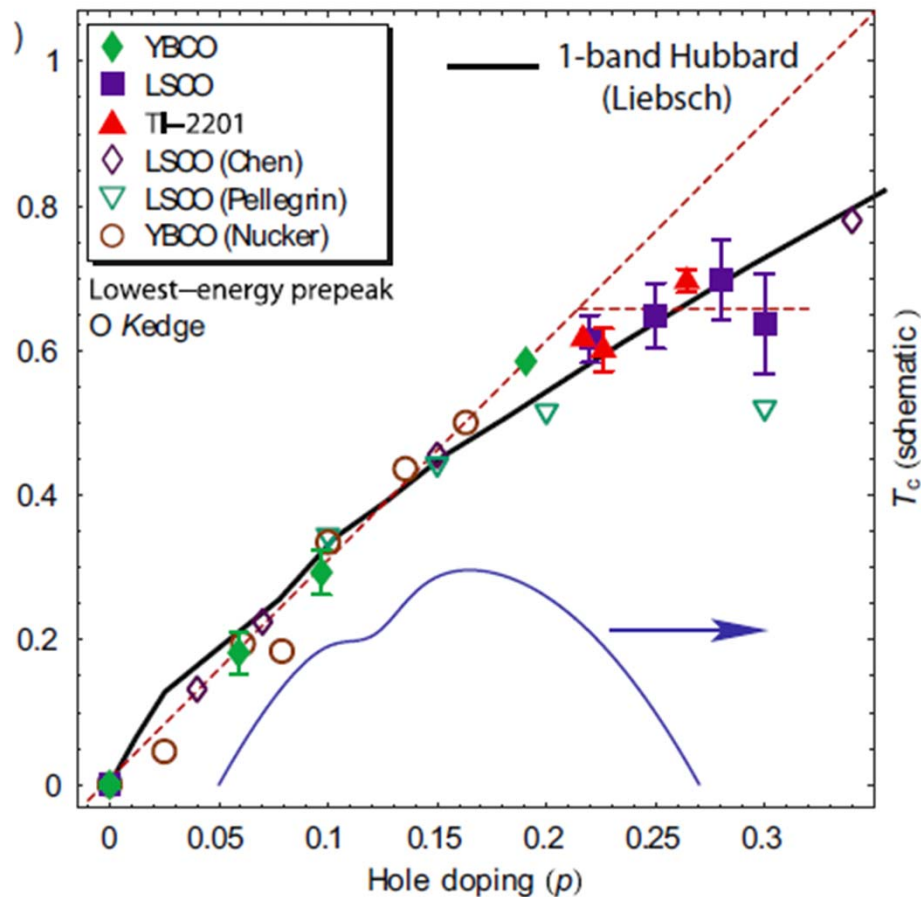


See also, Gull Millis, PRB, 2013



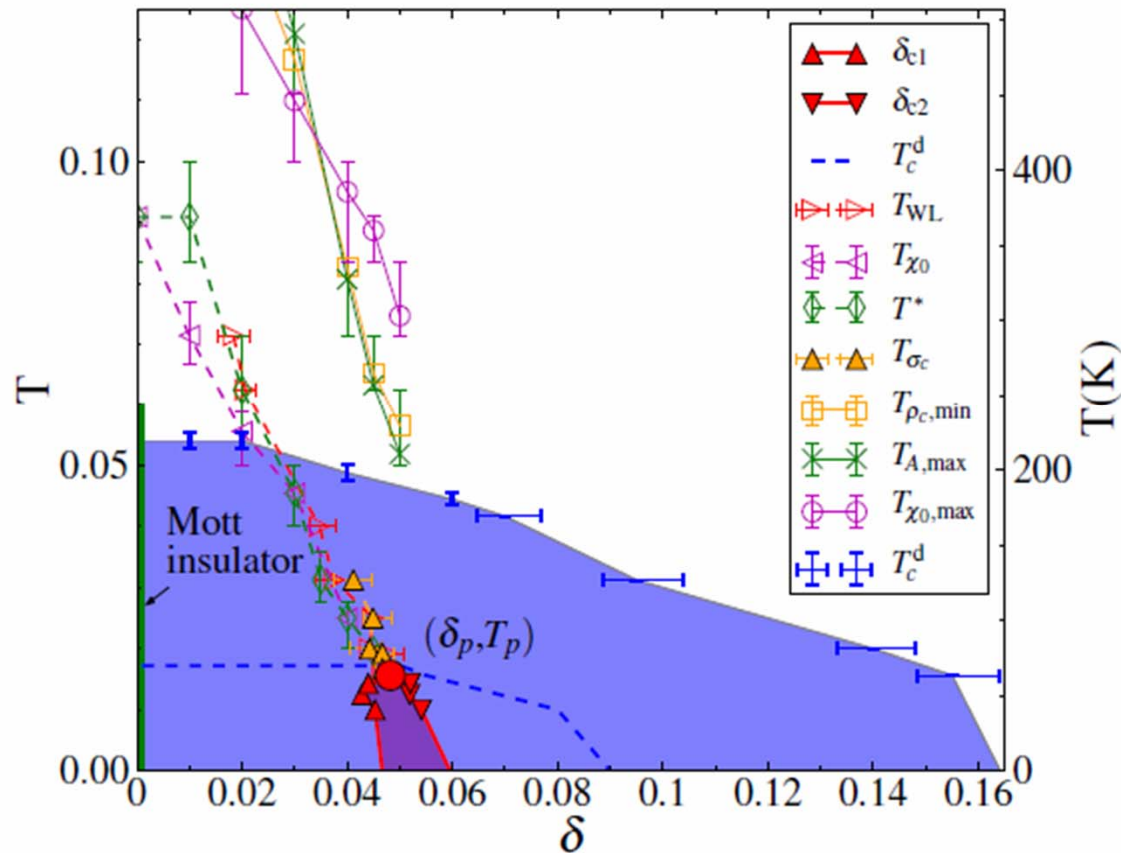
Panagopoulos et al. PRB 2000

Compare with number of carriers



Peets et al. PRL 2009, Phillips and Jarrell, PRL 2010

Phase diagram for $U = 6.2 t$

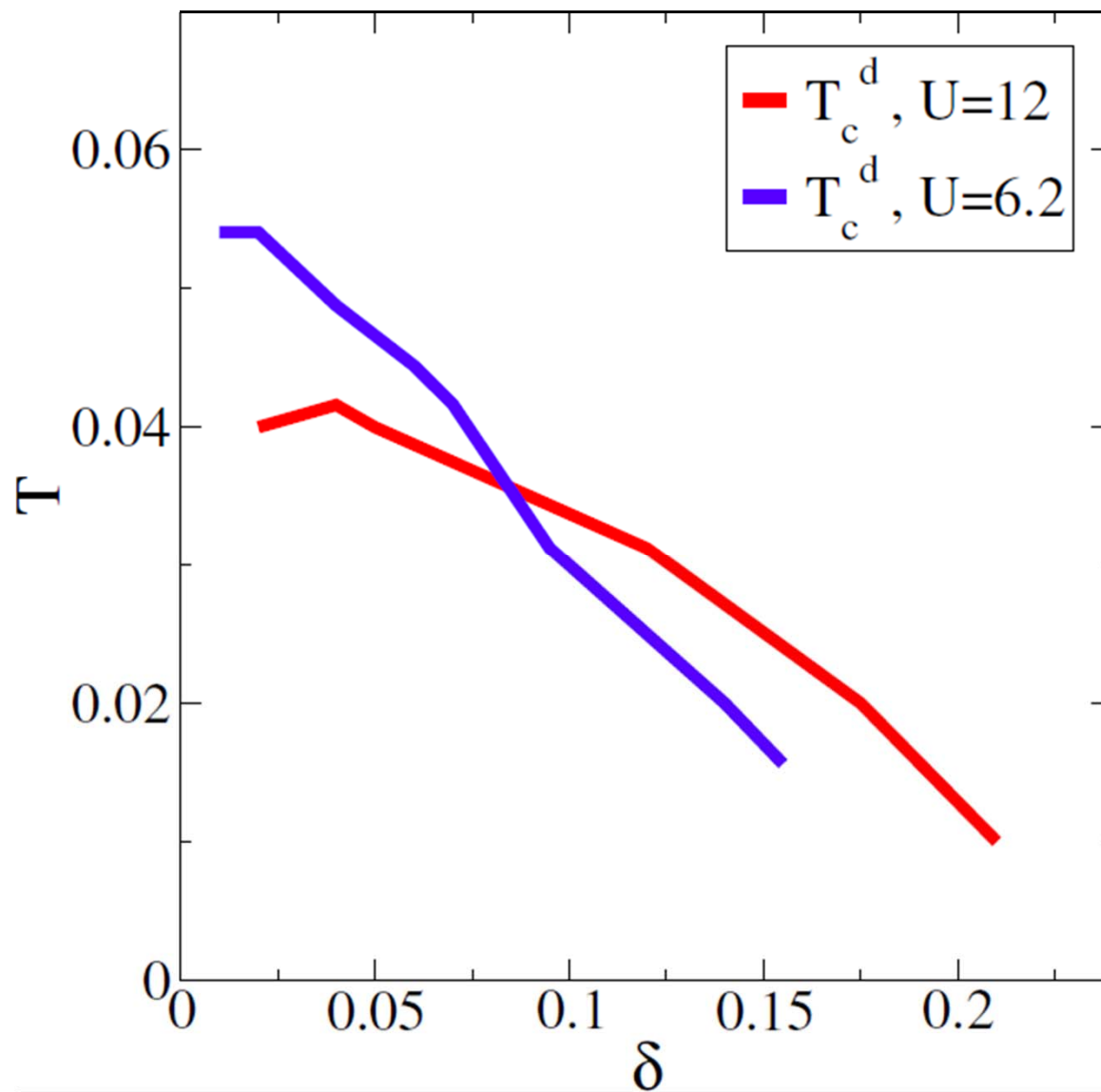


P. Sémon, G. Sordi, A.-M.S. Tremblay, [arxiv.org/1402.7087](https://arxiv.org/abs/1402.7087)



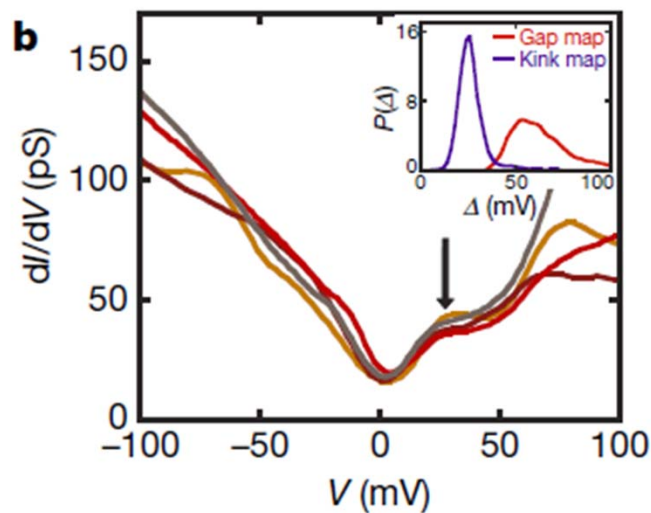
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$$T_c^d$$



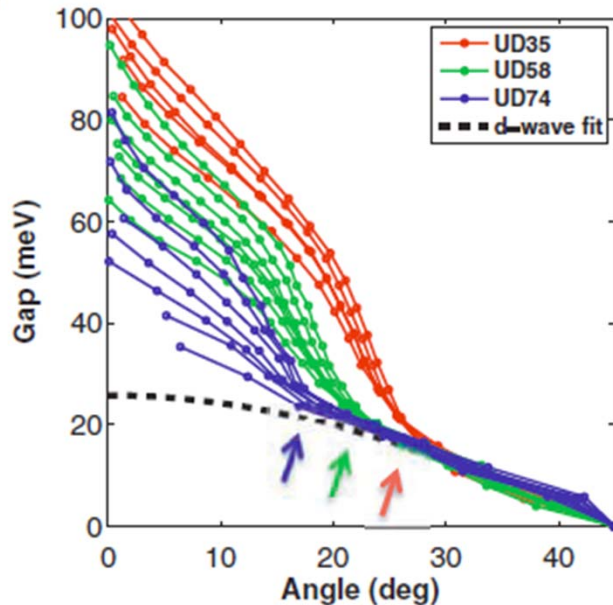
Meaning of T_c^d

- Local pair formation



K. K. Gomes, A. N. Pasupathy, A. Pushp,
S. Ono, Y. Ando, and A. Yazdani,
Nature **447**, 569 (2007)

Meaning of T_c^d : Local pair formation



A. Pushp, Parker, ... A. Yazdani,
Science **364**, 1689 (2009)

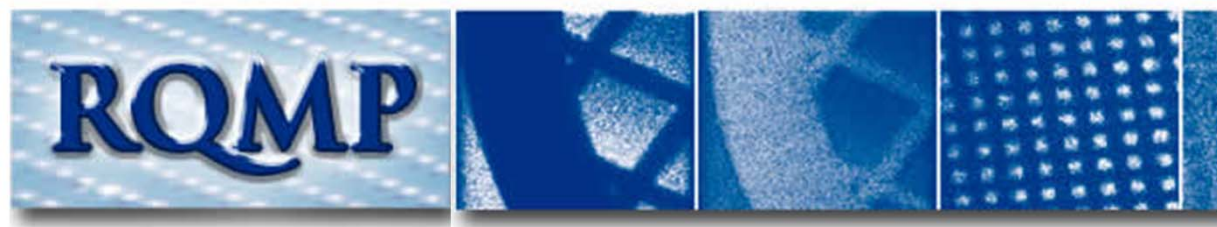
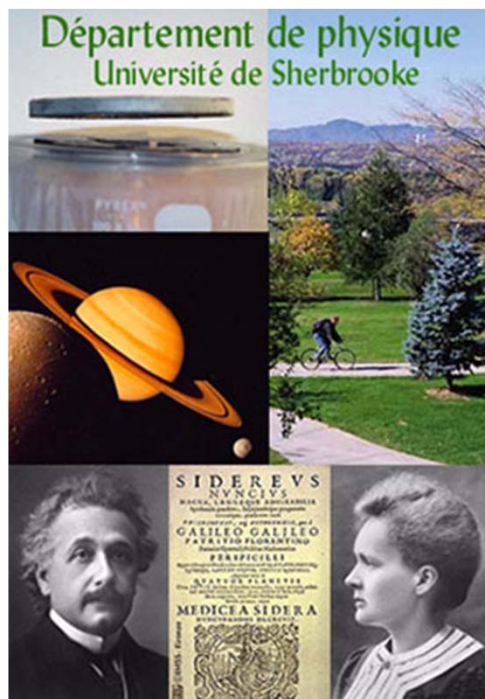
However, our measurements demonstrate that the nodal gap does not change with reduced doping. The pairing strength does not get weaker or stronger as the Mott insulator is approached; rather, it saturates.

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



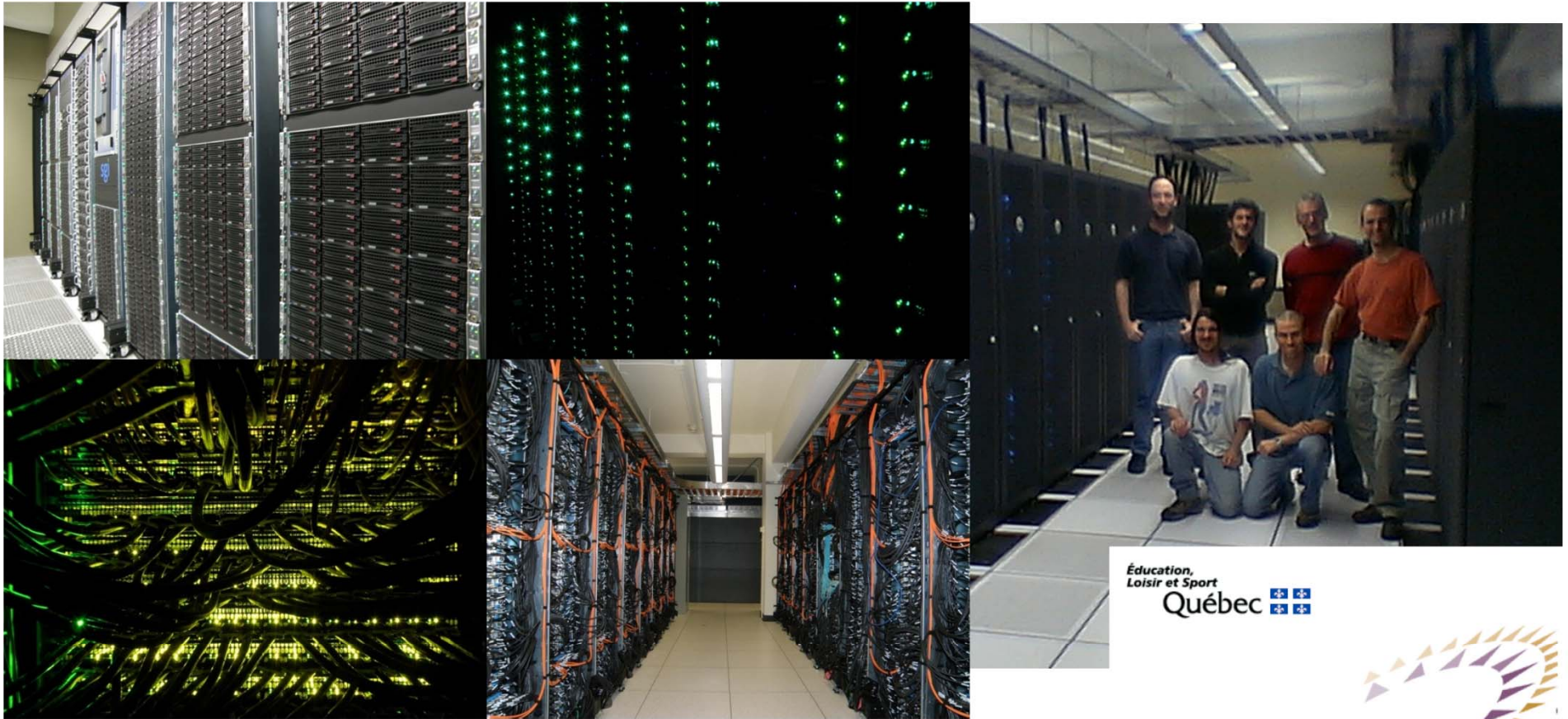
Le regroupement québécois sur les matériaux de pointe



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Le calcul de haute performance

CRÉER LE SAVOIR
ALIMENTER L'INNOVATION
BÂTIR L'ÉCONOMIE NUMÉRIQUE



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Merci

Thank you

Ergodicity of the hybridization expansion with two operator updates and broken symmetry

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

$$Z = \text{Tr} T_\tau e^{-\beta H_0} e^{-\int_0^\beta d\tau (H_{\text{hyb}}(\tau) + H_{\text{hyb}}^\dagger(\tau))} \\ = \sum_{k \geq 0} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau'_1 \cdots d\tau'_k \text{Tr} T_\tau e^{-\beta H_0} \\ \times H_{\text{hyb}}(\tau_1) H_{\text{hyb}}^\dagger(\tau'_1) \cdots H_{\text{hyb}}(\tau_k) H_{\text{hyb}}^\dagger(\tau'_k).$$

$$\text{Tr}[d_{\uparrow(0,\pi)} d_{\downarrow(0,\pi)} d_{\downarrow(\pi,0)}^\dagger d_{\uparrow(\pi,0)}^\dagger] \\ \times F_{\uparrow(0,\pi),\downarrow(0,\pi)} \overline{F}_{\uparrow(\pi,0),\downarrow(\pi,0)}$$