Antagonistic effects of nearest-neighbor repulsion on the superconducting pairing dynamics in the doped Mott insulator regime

A.-M.S. Tremblay,
A. Reymbaut, G. Sordi, D. Sénéchal

CECAM, 5 February 2019
Bremen

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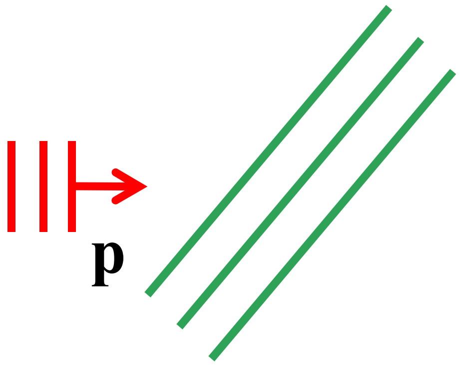
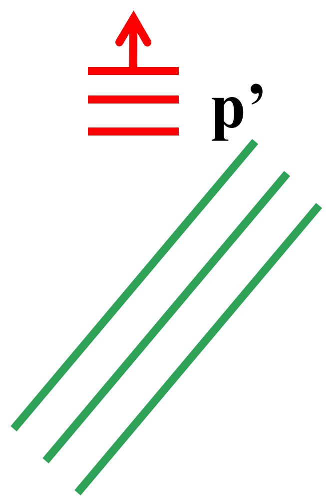
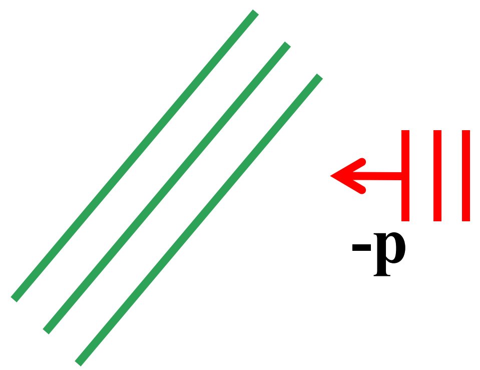
Attraction mechanism in the metallic state



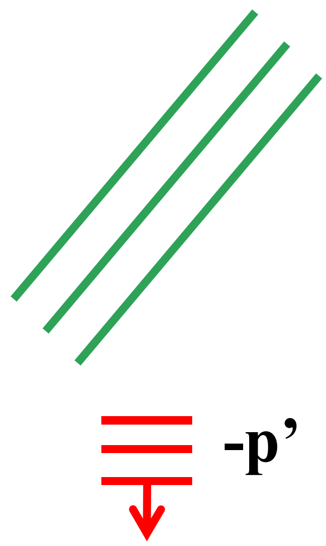
Attraction mechanism in the metallic state



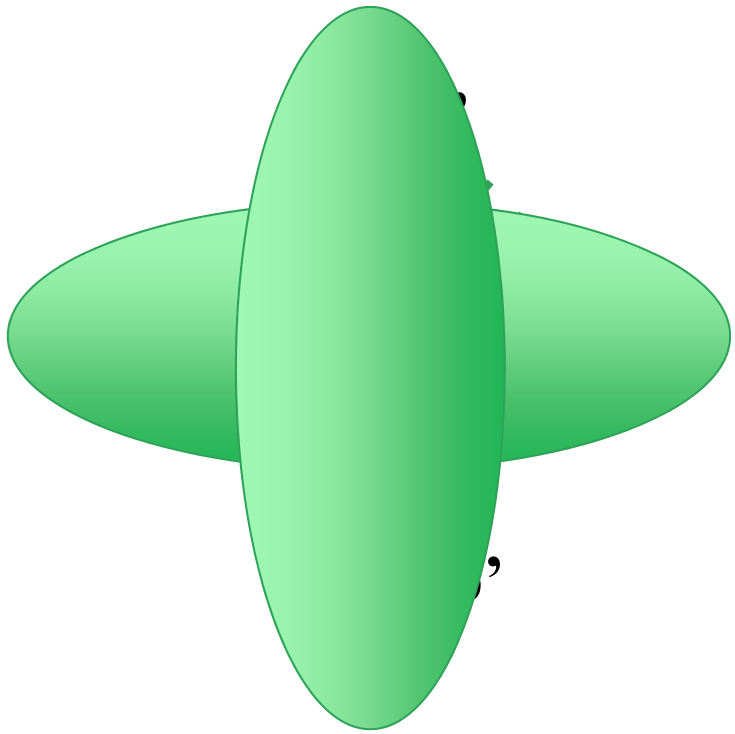
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow}$$

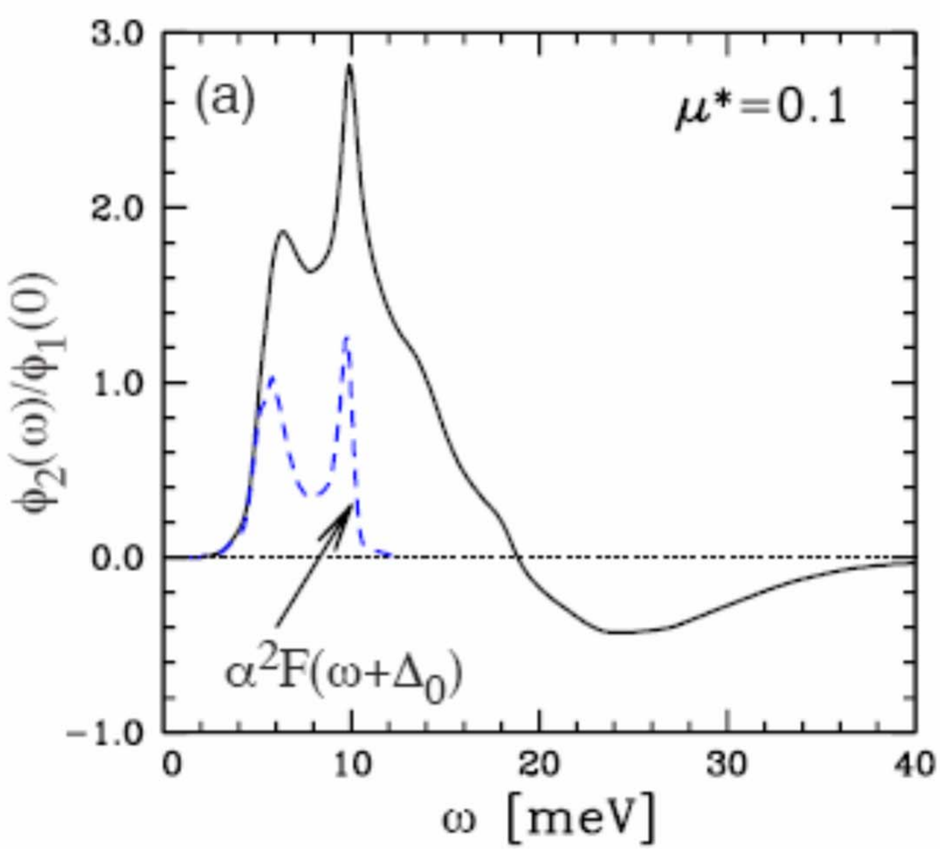
$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left\langle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \right\rangle \left\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \right\rangle$$

$$|\mathrm{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \ldots.$$

$$\varphi_{SC} = \langle c_{i\uparrow} c_{j\downarrow} \rangle$$

Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

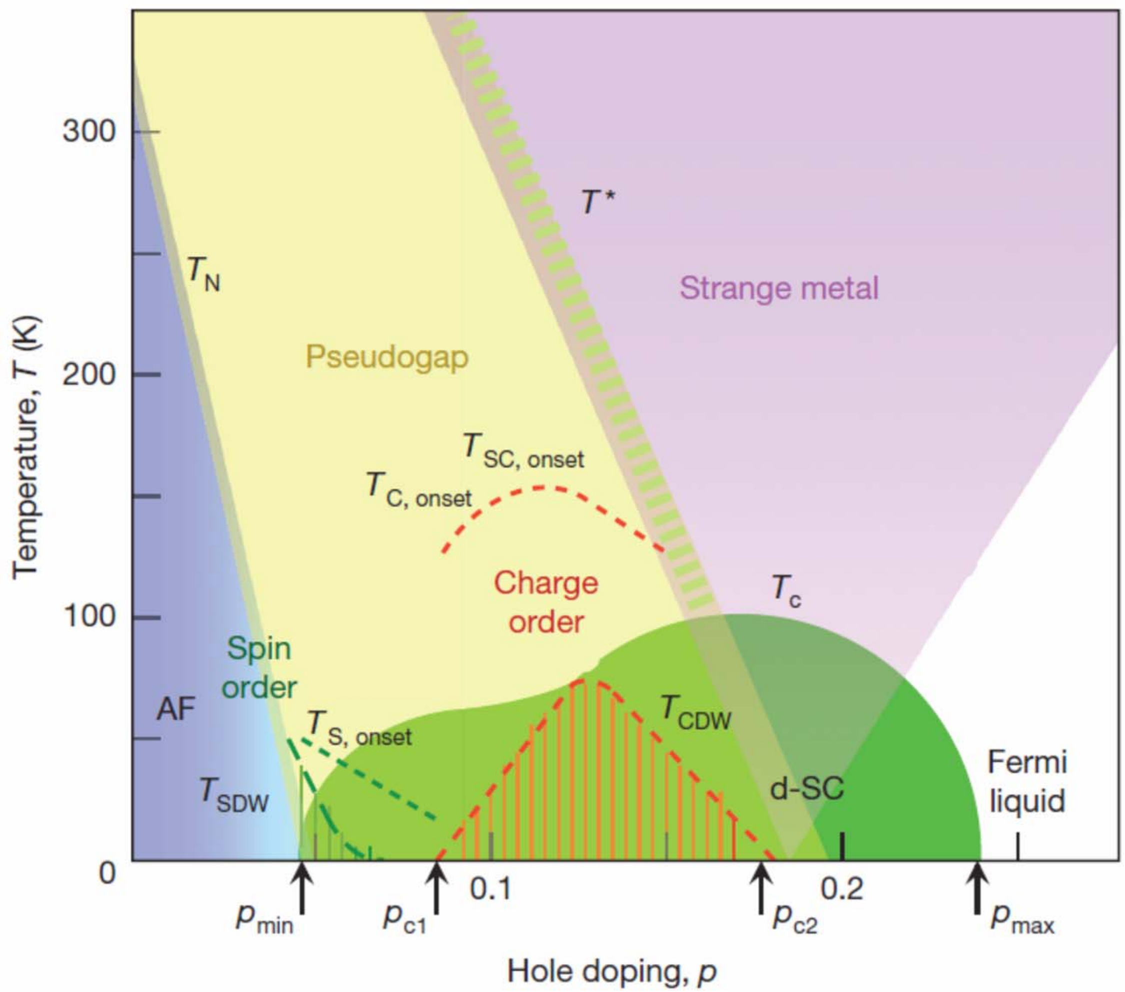


Retardation

μ^* in formulas for T_c

$$V_{eff} = \frac{V_c}{1 + N(0)V_c \ln\left(\frac{E_F}{\hbar\omega_D}\right)}$$ Anderson-Morel

Here: Phase diagram $YBa_2Cu_3O_{7-x}$

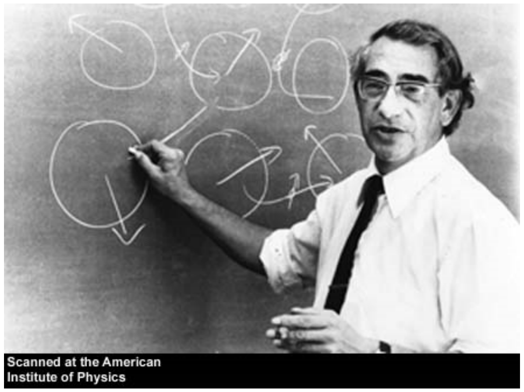


p or δ

Keimer et al., Nature 518, 179 (2015)

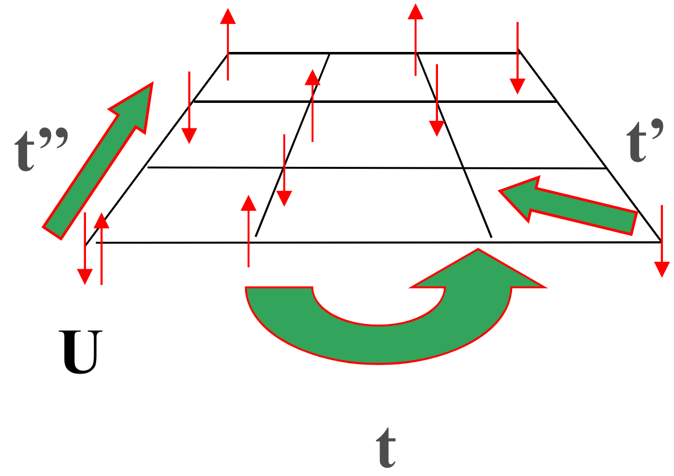
Model and question for this talk

Mott insulator: Hubbard Model



1931-1980

μ



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

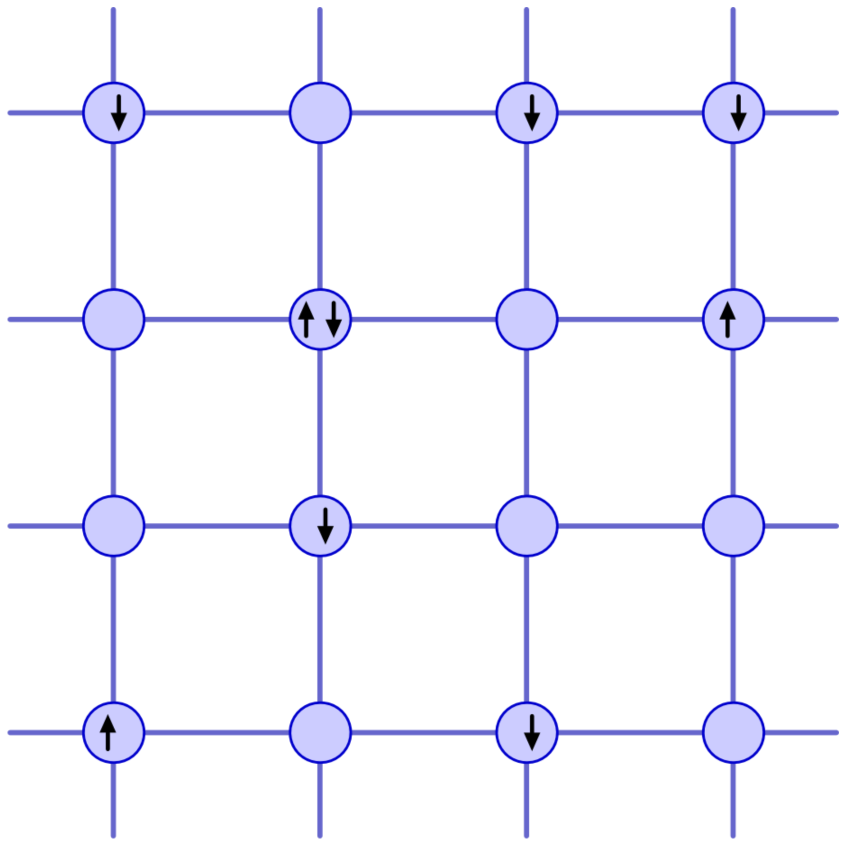
$t = 1,\ k_B = 1,\ \hbar = 1$

$$J\sum_{<i,j>} S_i \cdot S_j$$

$$J = \frac{4t^2}{U}$$

Attn: Charge transfer insulator

Extended Hubbard model



$$\hat{\mathcal{H}} = -t \sum_{\langle i,j \rangle \; \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + c.h \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i$$

Effect of near-neighbor repulsion *V*

$$\hat{\mathcal{H}}_{Hubbard} = -\sum_{\langle i,j\rangle_{1,2,3}\ \sigma}\left(t_{ij}\,\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + c.h\right) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + V\sum_{\langle i,j\rangle}\hat{n}_i\hat{n}_j - \mu\sum_{i\ \sigma}\hat{n}_{i\sigma}$$

$YBa_2Cu_3O_7$: $t=1$ $t'=-0.3$ $t''=0.2$

Superconductivity disappears when:

$$V > U\frac{U}{W}$$

In weakly correlated case
U/W < 1

S. Raghu, E. Berg, A. V. Chubukov et S. A. Kivelson, PRB **85**, 024516 (2012)

S. Onari, R. Arita, K. Kuroki et H. Aoki, PRB **70**, 094523 (2004)

Effect of near-neighbor repulsion V

In strongly correlated case, superconductivity disappears when

$$V > 4J$$

In cuprates:

$$V = 400\,\mathrm{meV}$$

$$J = 130\,\mathrm{meV}$$

Yes

S. Zhou *et al*. Phys. Rev. B **70** (2004)
R. M. Noack *et al*. Europhys. Lett. **30** (1995)
R. M. Noack *et al*. Phys. Rev. B **56** (1997)
E. Arrigoni *et al*. Phys. Rev. B **65** (2002)

No

E. Plekhanov, S. Sorella, *et al*. Phys. Rev. Lett. **88**, 117002 (2002)
D. Sénéchal *et al*. Phys. Rev. B **87** (2013)
A. Reymbaut *et al*. Phys. Rev. B **94** (2016)
M. Jiang .. T. Maier *et al*. Phys. Rev. B **97** (2018)

Outline

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APOGÉE CANADA
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Outline

I. Method
II. Phase diagram at $V = 0$
III. Antagonistic effects of V
IV. Diagnostics for retardation
V. Differences between weak and strong correlations superconductivity
VI. Conclusion

I. Method

- Dynamical Mean Field Theory
  – clusters
- Concept: atomic-like localized correlations consistent with delocalized aspect

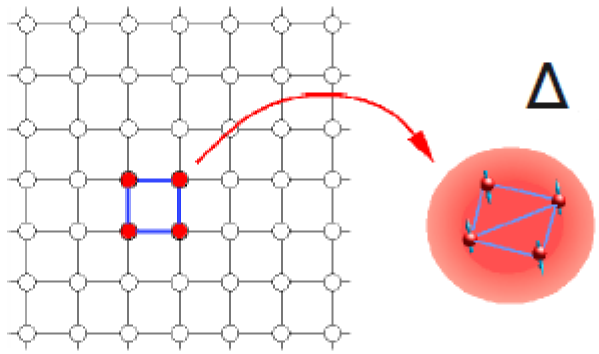
REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

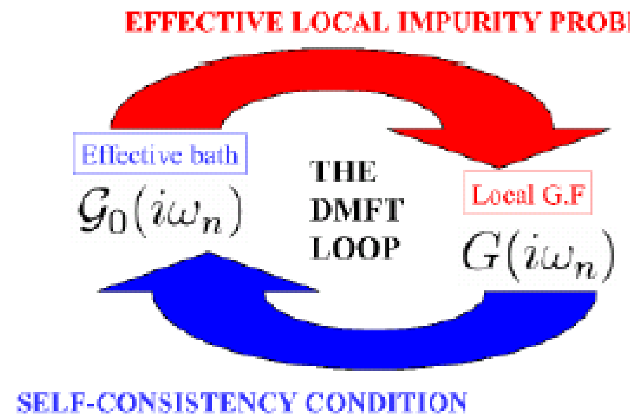
Hettler *et al*, PRB 1998
Lichtenstein *et al.*,PRB 2000
Kotliar *et al.*, PRB 2000
M. Potthoff, EJP 2003

Cellular DMFT + CT-QMC

E. Gull, A J. Millis, A. I. Lichtenstein, A. N. Rubtsov. M. Troyer. P. Werner, RMP **83**, 350 (2011)

$$Z = \int D[d^\dagger, d] \exp\left[-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i [d_i^\dagger(\tau) \Delta_{i' i}(\tau, \tau') d_{i'}(\tau')] \right]$$





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

Algorithmic improvements for CT-HYB

P. Sémon *et al.*

4 point updates for ergodicity in SC state: PRB **90** 075149 (2014);

Lazy skip list for fast cluster trace: PRB **89**, 165113 (2014)

Patrick Sémon

+ and -

- Long range order:
  - No mean-field factorization on the cluster
  - Symmetry breaking allowed in the bath (mean-field)
- Included :
  - Short-range dynamical and spatial correlations
  - V exactly in the cluster, in mean-field between clusters
- Missing:
  - Long wavelength p-h and p-p fluctuations

Some groups using these methods for cuprates

- Europe:
  - Georges, Parcollet, Ferrero, Civelli, Wu (Paris)
  - Lichtenstein, Potthoff, (Hamburg) Aichhorn (Graz), Liebsch (Jülich) de Medici (Grenoble) Capone (Italy)
- USA:
  - Gull (Michigan) Millis (Columbia)
  - Kotliar, Haule (Rutgers)
  - Jarrell (Louisiana)
  - Maier, Okamoto (Oakridge)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome

Maximum entropy analytic continuation of non-positive spectral weights

A. Reymbaut, D. Bergeron, and A.-M. S. T. Phys. Rev. B **92**, 060509(R) (2015)

$$\mathcal{F}(\vec{k},i\omega_n) = -\int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau} \langle \hat{\mathcal{T}}_\tau\, \hat{c}_{\vec{k}\uparrow}(\tau)\, \hat{c}_{-\vec{k}\downarrow}(0)\rangle_{\hat{\mathcal{H}}} \, .$$

$$\mathcal{G}_{aux}(\vec{k},\tau) = -\langle \hat{\mathcal{T}}_\tau\, \hat{a}_{\vec{k}}(\tau)\, \hat{a}^\dagger_{\vec{k}}(0)\rangle_{\hat{\mathcal{H}}},$$

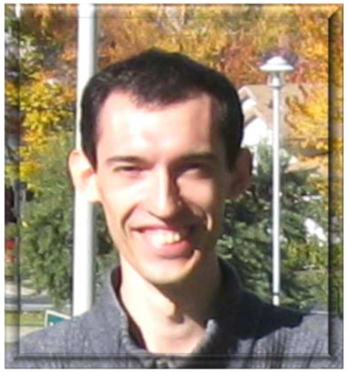
$$\hat{a}_{\vec{k}} = \hat{c}_{\vec{k}\uparrow} + \hat{c}^\dagger_{-\vec{k}\downarrow}$$

$$\mathcal{G}_{aux}(\vec{k},i\omega_n) = \mathcal{G}_\uparrow(\vec{k},i\omega_n) - \mathcal{G}_\downarrow(\vec{k},-i\omega_n) + 2\mathcal{F}(\vec{k},i\omega_n),$$

OmegaMaxEnt:

Dominic Bergeron and A.-M. S. T., Phys. Rev. E **94,** 023303 (2016).

II.
Phase Diagram V = 0



Giovanni Sordi

Lorenzo Fratino

Patrick Sémon

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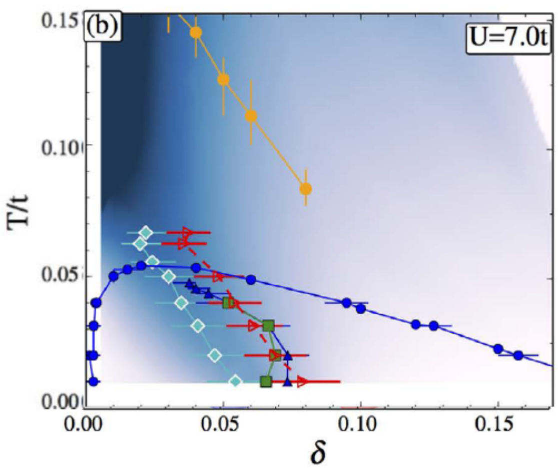
Phase diagram, *V = 0*

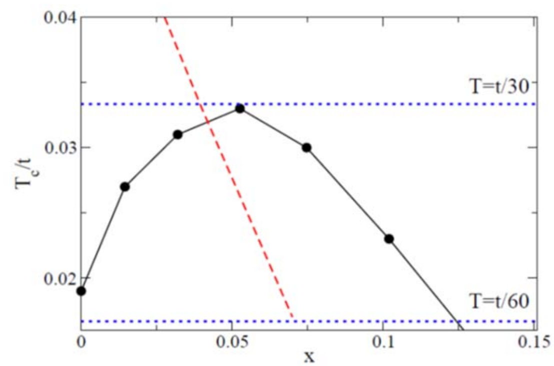
4 sites



Fratino et al.
Sci. Rep. **6**, 22715

U = 7

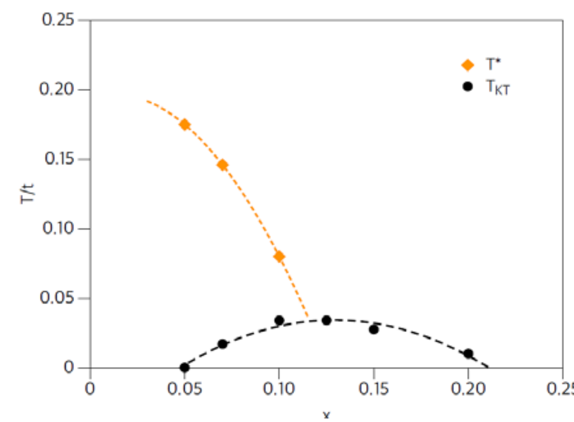
8 sites



E. Gull and A. J. Millis
Phys. Rev. B 88, 075127

U = 6

12 sites

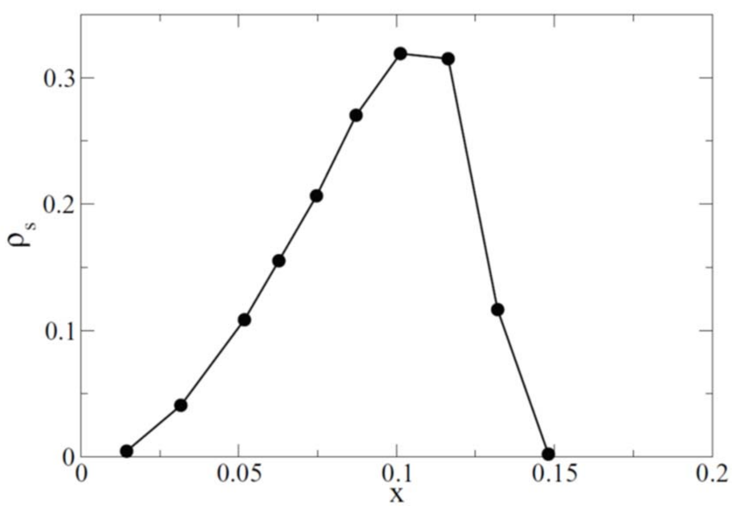


T. Maier D. J Scalapino
arxiv.org/1810.10043

U = 7

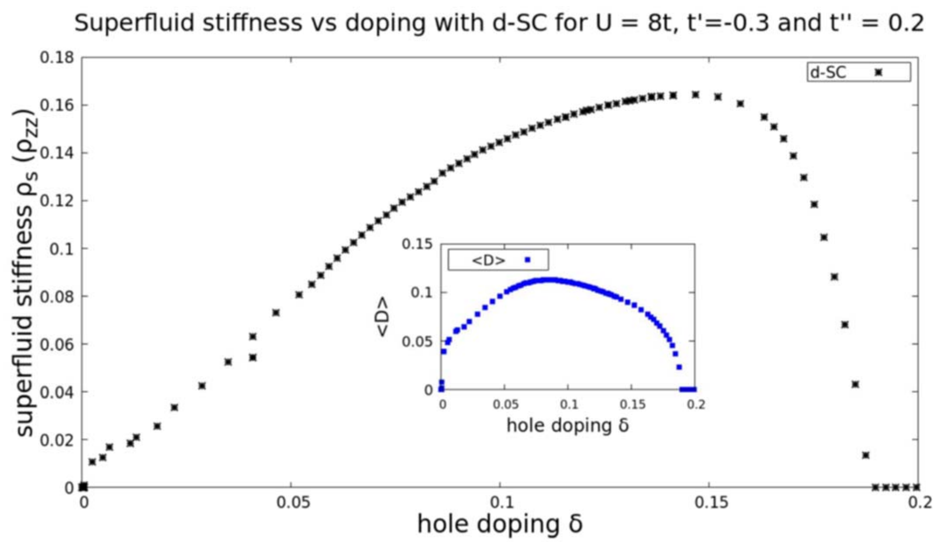
Superfluid stiffness and phase fluctuations

U = 6, *T*=1/60, 8 sites

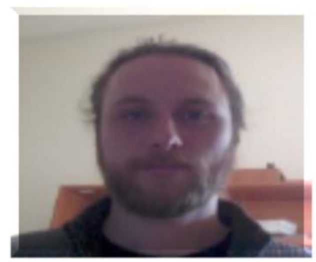


E. Gull and A. J. Millis
Phys. Rev. B 88, 075127

U = 8, *T*=0, 4 *sites*



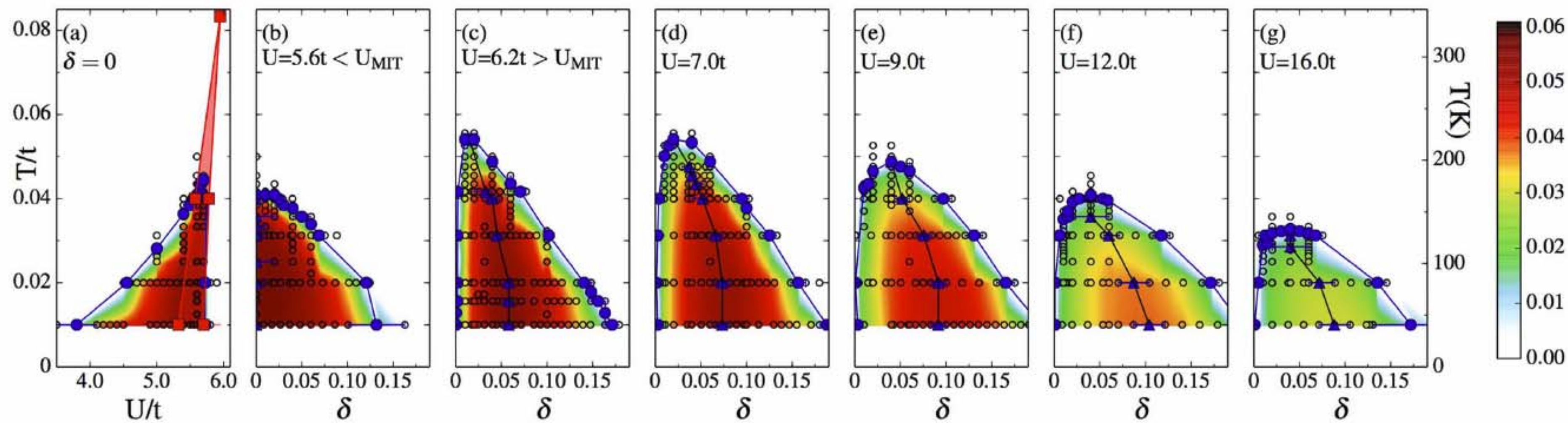
Olivier Simard



Alexandre Foley

David Sénéchal

T_c controlled by J



Fratino et al.
Sci. Rep. **6**, 22715

$$\varphi_{SC} = \langle c_{i\uparrow} c_{j\downarrow} \rangle$$

Some experiments that suggest $T_c < T_{pair} < T^*$

T. Kondo *et al*. PRL **111** (2013)

Kondo, Takeshi, et al. Kaminski Nature Physics 2011, *7*, 21-25

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

Lee …Tajima (Osaka) https://arxiv.org/pdf/1612.08830

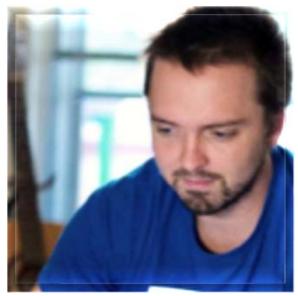
Patrick M. Rourke, et al. Hussey Nature Physics **7,** 455–458 (2011)

Lee et al. J. Phys. Soc. Jpn. 86, 023701 (2017)

Alexis Reymbaut

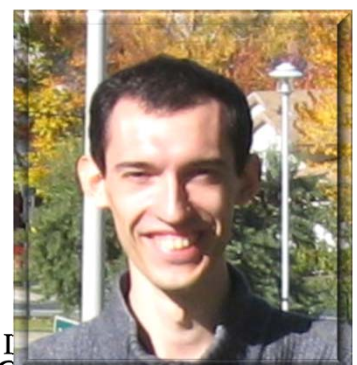
III. Antagonistic effects of *V*

Marco Fellous Assiani



Maxime Charlebois

Patrick Sémon



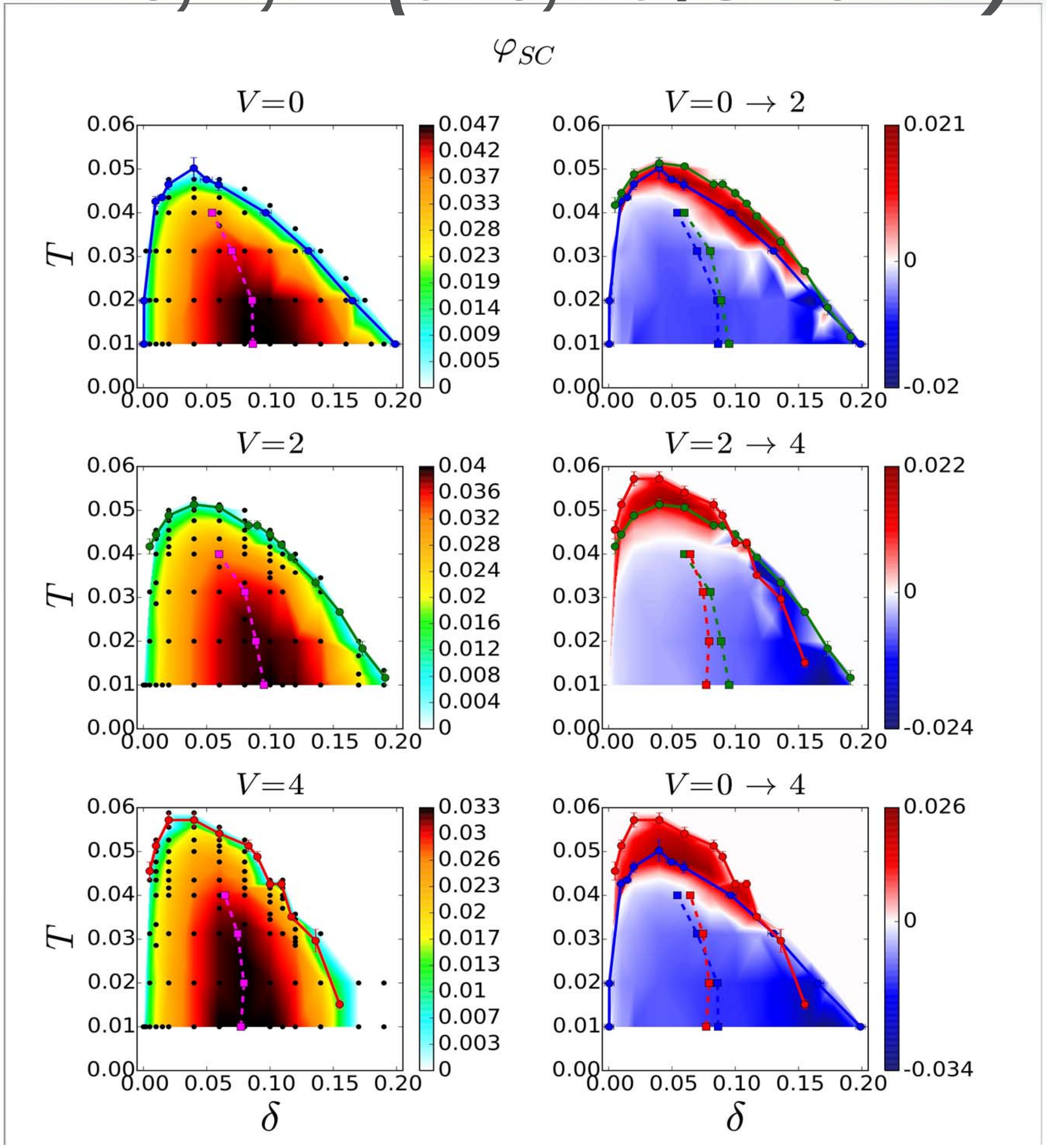
Giovanni Sordi

Lorenzo Fratino

U = 9, V = 0, 2, 4 (t'=0, $4t^2/U$ ~0.44)

$$\varphi_{SC} = \langle c_{i\uparrow} c_{j\downarrow} \rangle$$

A. Reymbaut *et al.*
PRB **94**, 155146



IV.
Is retardation playing a role? Diagnostics

Th. Maier, D. Poilblanc, D.J. Scalapino, PRL (2008)

M. Civelli, PRL **103**, 136402 (2009)

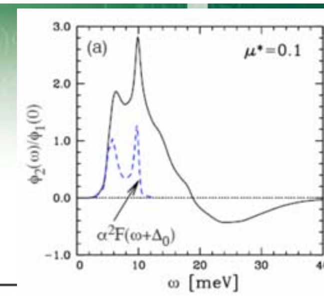
M. Civelli PRB 79, 195113 (2009)

E. Gull, A. J. Millis PRB **90**, 041110(R) (2014)

S. Sakai, M. Civelli, M. Imada PRL **116**, 057003 (2016)

The glue and neutrons, *V = 0*, *U=8, T=0*

Kyng, Sénéchal, AMST, PRB **80**, 205109 (2009)



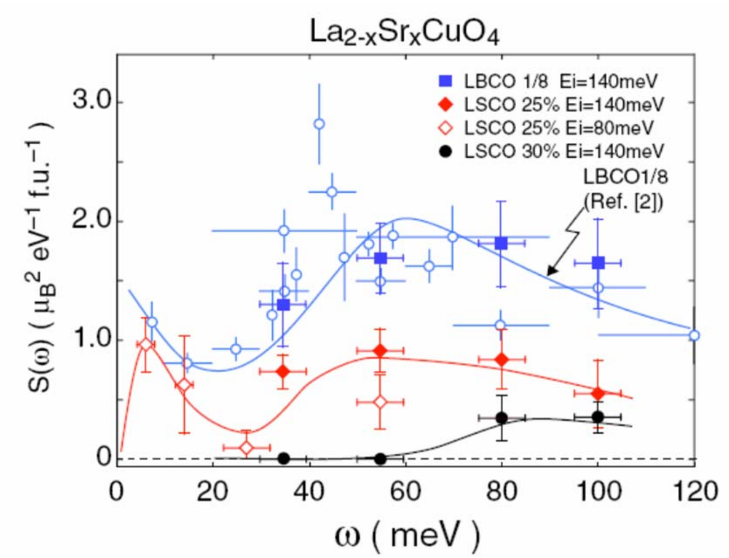
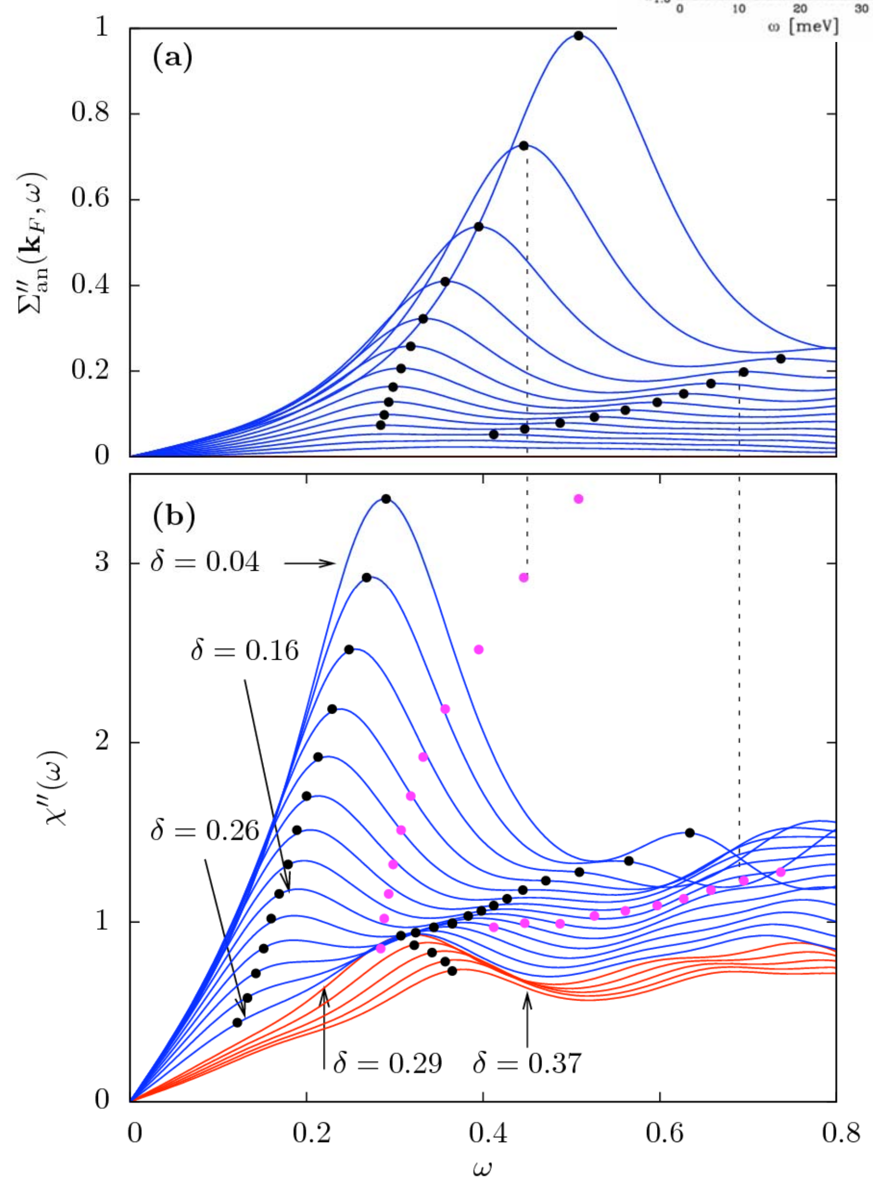


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.



Wakimoto … Birgeneau PRL (2007); PRL (2004)

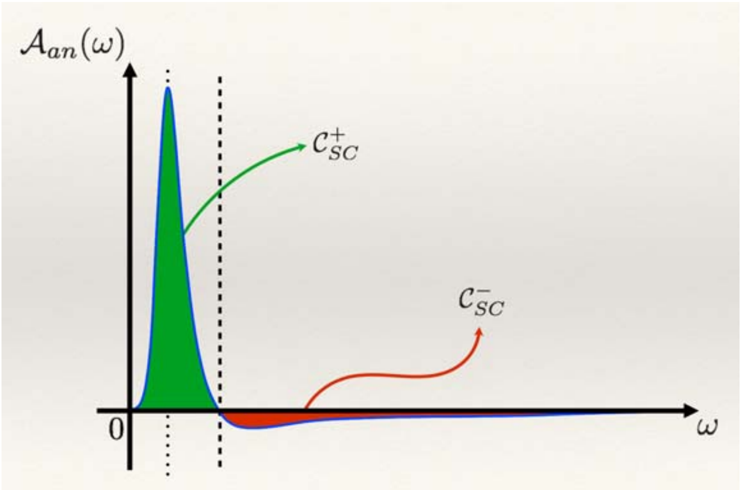
Frequencies important for pairing

Anomalous Green function

$$[\mathcal{F}_{an}(t)]_{lm} = -i\theta(t)\left\langle\{\hat{c}_{l\uparrow}(t), \hat{c}_{m\downarrow}(0)\}\right\rangle_{\mathcal{H}_{AIM}}$$

Anomalous spectral function

$$[\mathcal{A}_{an}(\omega)]_{lm} = -\frac{1}{\pi}\,\mathrm{Im}\,[\mathcal{F}_{an}(\omega)]_{lm}$$



Frequencies important for pairing

$V = 0$, $U=8$, $T=0$

David Sénéchal

Bumsoo Kyung

Anomalous Green function

$$[\mathcal{F}_{an}(t)]_{lm} = -i\theta(t)\left\langle\{\hat{c}_{l\uparrow}(t), \hat{c}_{m\downarrow}(0)\}\right\rangle_{\mathcal{H}_{AIM}}$$

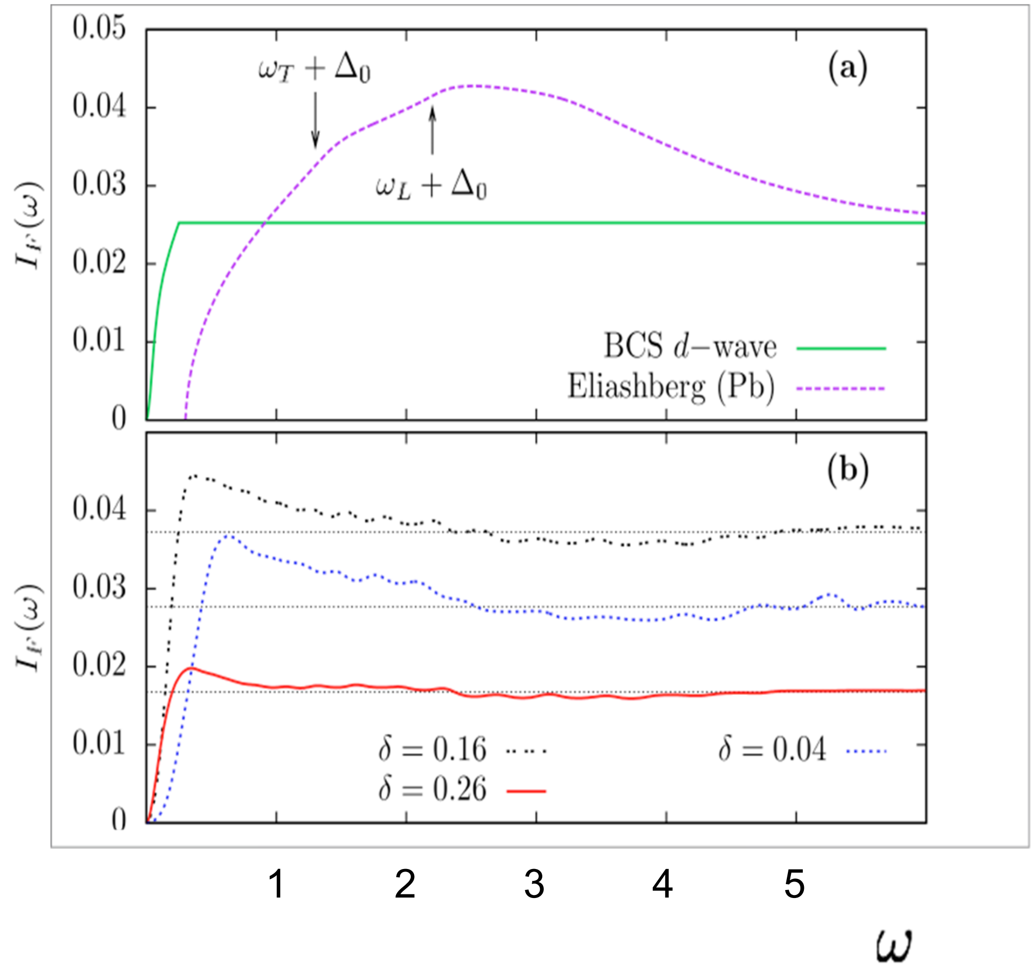
Anomalous spectral function

$$[\mathcal{A}_{an}(\omega)]_{lm} = -\frac{1}{\pi}\,\mathrm{Im}\,[\mathcal{F}_{an}(\omega)]_{lm}$$

Cumulative order parameter:

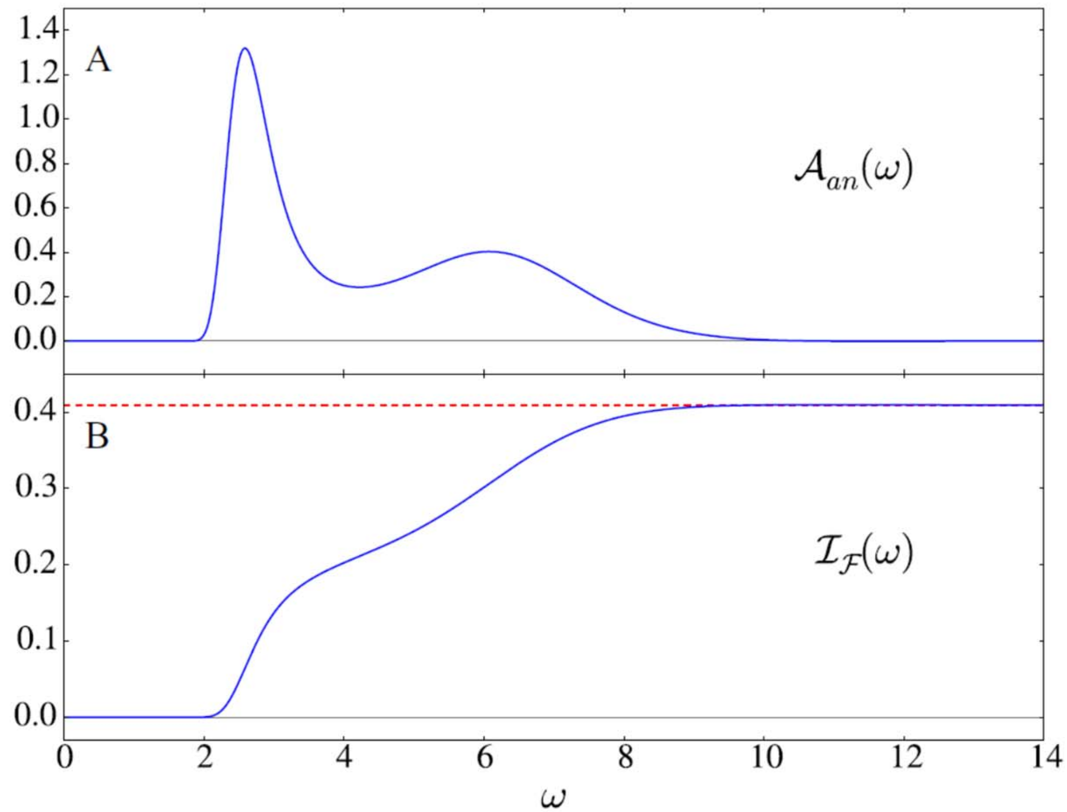
$$I_{\mathcal{F}}(\omega) = -\int_0^{\omega}\frac{\mathrm{d}\omega'}{\pi}\,\mathrm{Im}\,[\mathcal{F}_{an}(\omega')]_{lm}$$

$$I_{\mathcal{F}}(\omega) \xrightarrow[\omega\to+\infty]{} \langle\hat{c}_{l\uparrow}\hat{c}_{m\downarrow}\rangle_{\mathcal{H}_{AIM}}$$



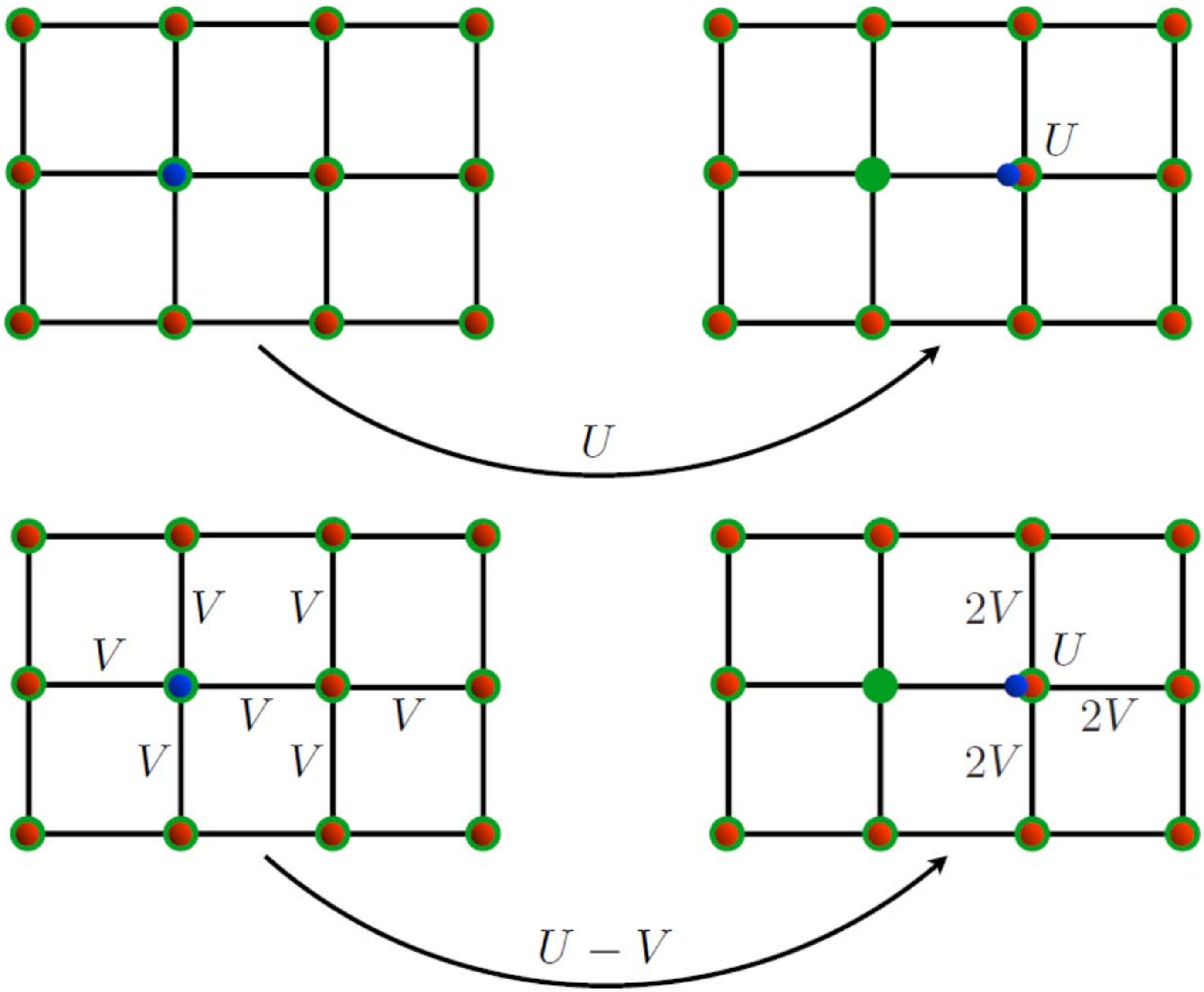
Scalapino, Schrieffer, Wilkins,
Phys. Rev. **148** (1966)

Contrast *U = -9, V = 0, s-wave*

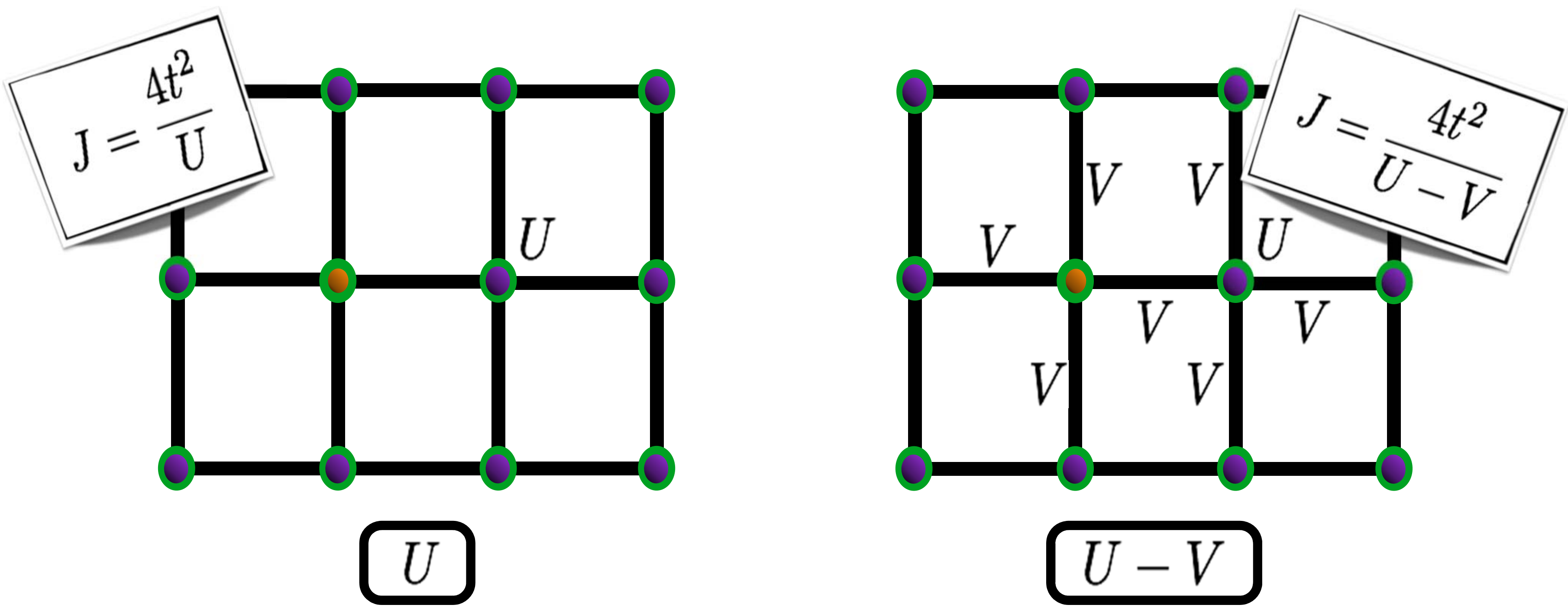


Introduce V

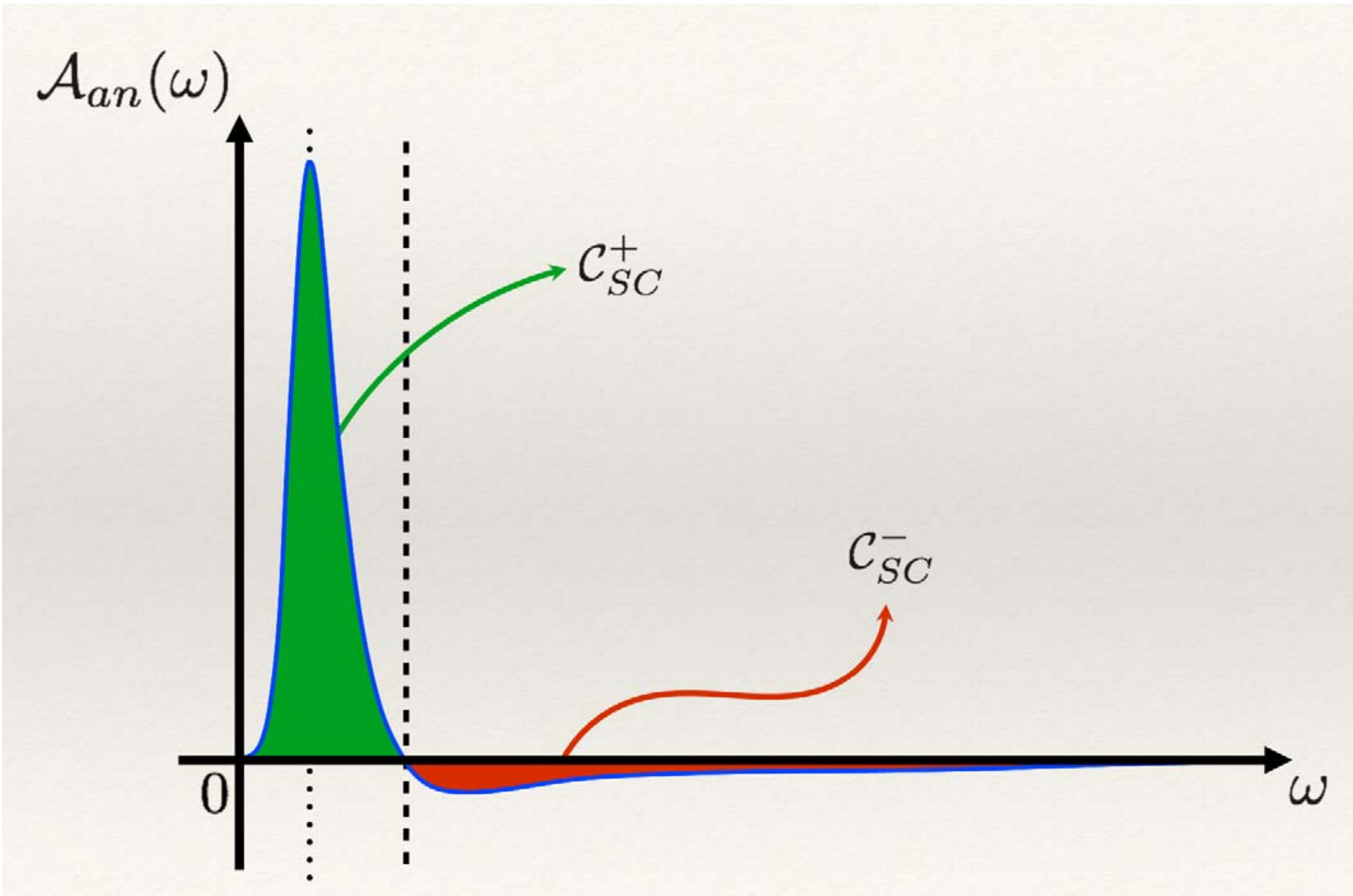
V also increases *J*



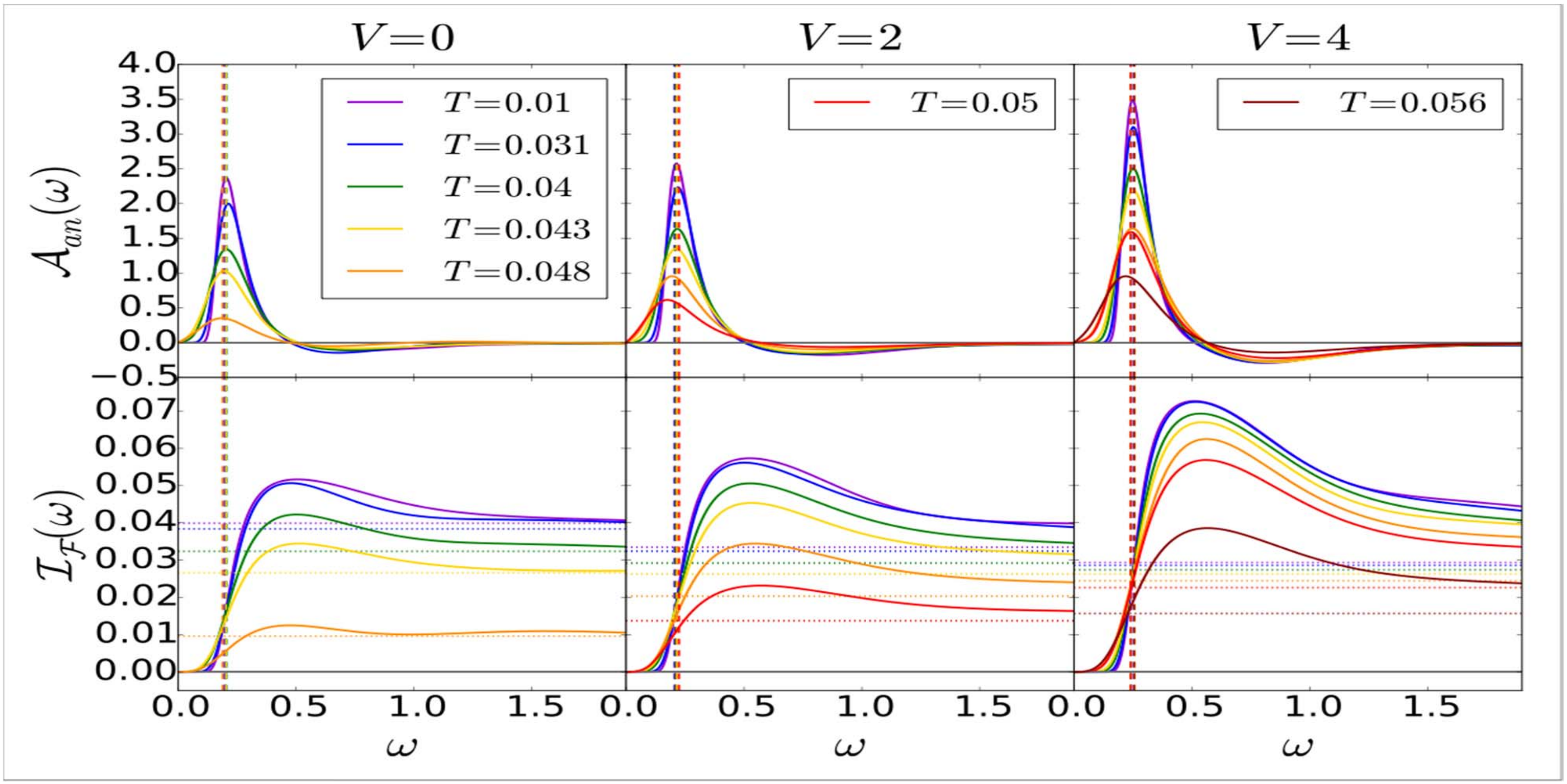
V also increases *J*



Positive and negative contributions



Pairing and depairing for $\delta = 0.04,\ \mathrm{U} = 9$

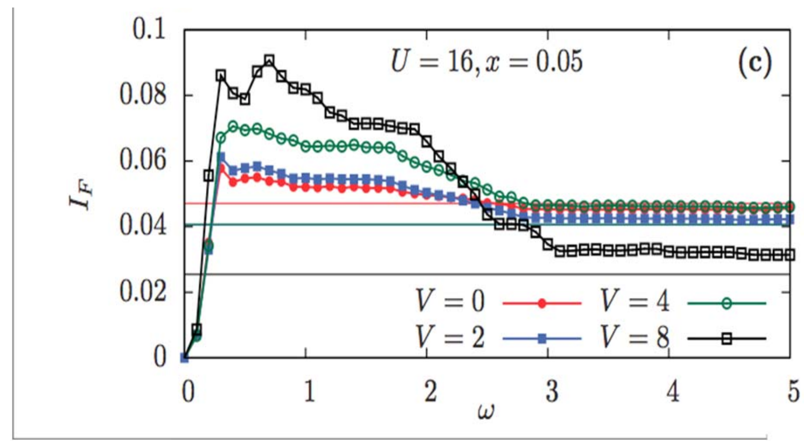


Binding aspects of V at $T = 0$

$$J = \frac{4t^2}{U - V}$$

***J* increases with *V* explaining better pairing at low frequency**

But V also induces more repulsion at high frequency, explaining the negative impact at high frequency on binding

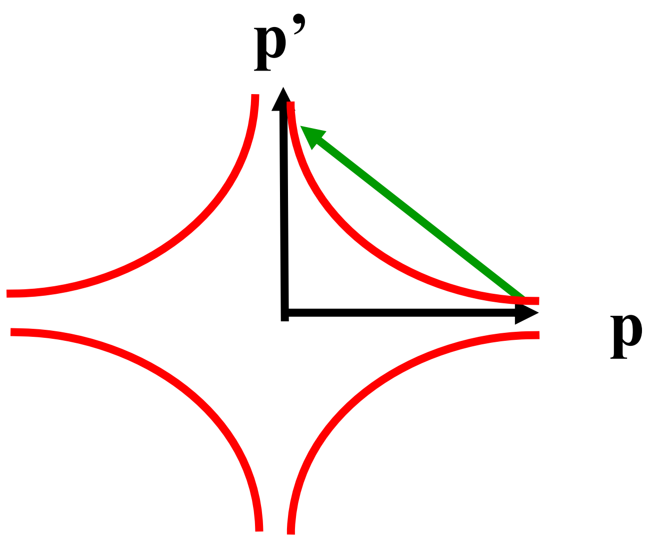


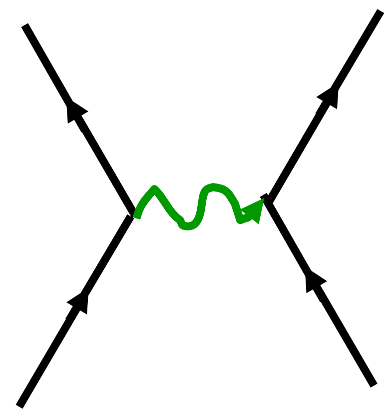
Sénéchal, Day, Bouliane, AMST, Phys. Rev. B **87**, 075123 (2013)

V.
Different pairing physics at weak and strong correlations

Cartoon « BCS » weak-correlation picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V}\sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right)$$





Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

Béal–Monod, Bourbonnais, Emery P.R. B. **34**, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch P.R. B **34**, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. **15**, 524 (1965).

P.W. Anderson Science 317, 1705 (2007)

A cartoon strong correlation picture

$$J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle i,j \rangle} \left(\frac{1}{2} c_i^\dagger \vec{\sigma} c_i \right) \cdot \left(\frac{1}{2} c_j^\dagger \vec{\sigma} c_j \right)$$

$$d = \langle \hat{d} \rangle = 1/N \sum_{\vec{k}} (\cos k_x - \cos k_y) \langle c_{\vec{k},\uparrow} c_{-\vec{k},\downarrow} \rangle$$

$$H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^\dagger) + F_0$$

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

P.W. Anderson Science 317, 1705 (2007)

Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

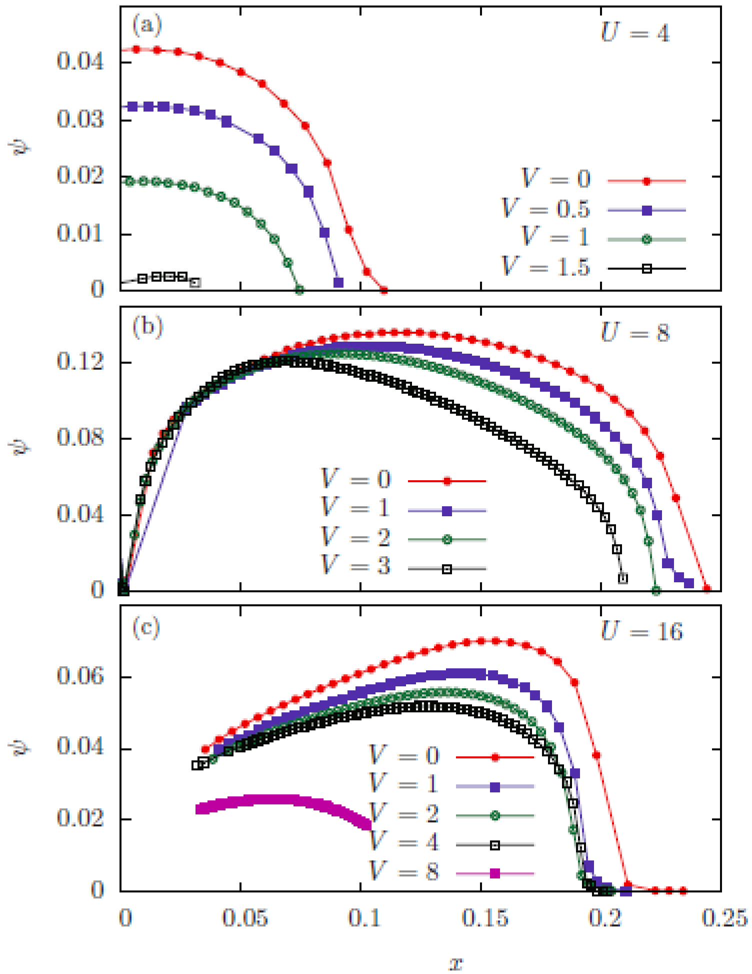
Resilience to near-neighbor repulsion

$$\varphi_{SC} = \langle c_{i\uparrow} c_{j\downarrow} \rangle$$

David Sénéchal

Alexandre Day

Vincent Bouliane

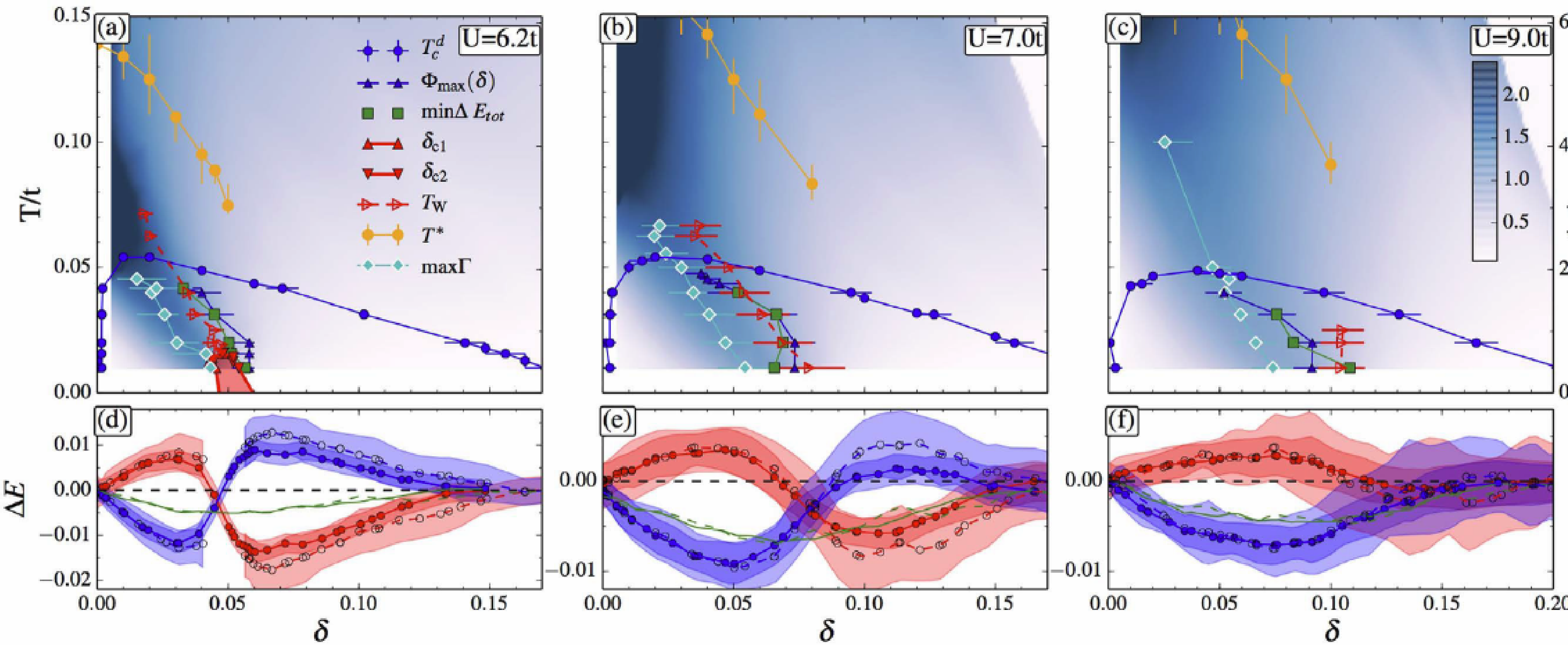


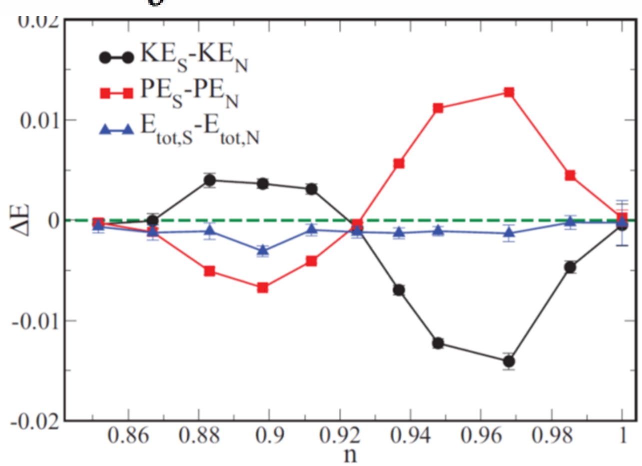
YBCO, T=0

$$J = 0.25, 4J = 1$$
$$V = 8$$

Sénéchal, Day, Bouliane, AMST PRB **87**, 075123 (2013)

Potential or kinetic energy driven?





Fratino et al.
Sci. Rep. **6**, 22715

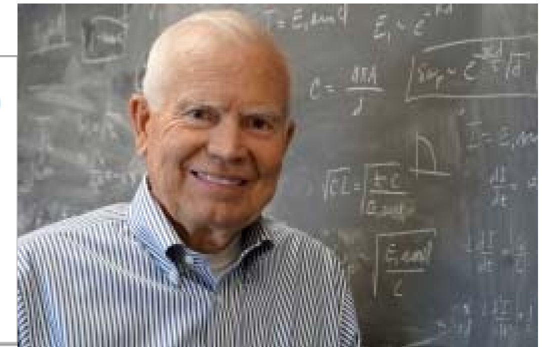
E.Gull and A.J. Millis PRB **86**, 241106(R) (2012)

Raising the question of the glue

D.J. Scalapino

P.W. Anderson

Is There Glue in Cuprate Superconductors?
Philip W. Anderson
Science **316**, 1705 (2007);
DOI: 10.1126/science.1140970



Is There Glue in Cuprate Superconductors?

Philip W. Anderson

Many theories about electron pairing in cuprate superconductors may be on the wrong track.

"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

Science e-letter, 5 and 10 Dec. 2007

Retardation

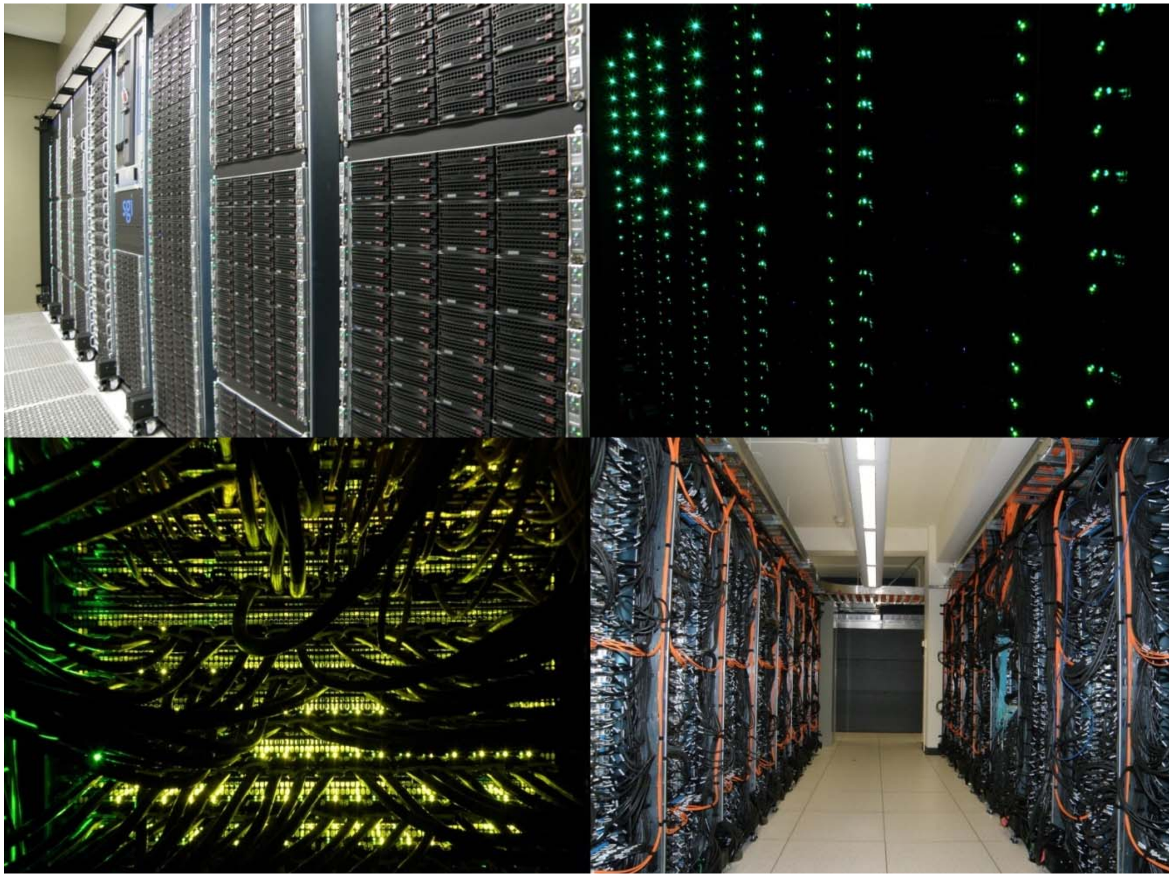
$$V^{eff}_{\acute{e}l-ph}(\vec{q},\omega) = \frac{e^2}{4\pi\varepsilon_0(q^2+k^2_{TF})}\left[1+\frac{\omega^2_{ph}(\vec{q})}{\omega^2-\omega^2_{ph}(\vec{q})}\right]$$

VI.
Conclusion

Conclusion

- Note: Increasing *V* leads to CDW instabilities not taken into account here
- The physics of pairing is retarded even for large interactions
- Like *U*, near-neighbor repulsion *V* is pair forming a low frequency (through J) and pair-breaking at high frequency.
- Pairing at large *U* (Strongly correlated superconductivity)
  - through *J* (short distance)
  - much more resilient to *V* than at small *U.*

Mammouth



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Calcul Québec

Merci
Danke
Thank you

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