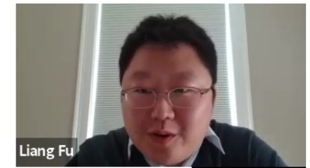
Title: 3-particle mechanism for pairing and superconductivity

Speakers: Liang Fu
Date: April 19, 2021 - 12:30 PM

URL: http://pirsa.org/21040011

Abstract: I will present a new mechanism for superconductivity from strong electron-electron repulsion in multi-band systems. When the kinetic energy is small, the dynamics of nearby electrons on the lattice is strongly correlated. I will introduce a controlled expansion in the kinetic term to demonstrate pairing induced by correlated tunneling process involving a third electron in the occupied band. This mechanism can also be viewed as the real space picture of exciton-mediated pairing. Possible realization of this idea leading to strong-coupling, spin-triplet superconductivity in WTe2 and magic-angle graphene will be discussed.

Based on works with Valentine Crepel and Kevin Slagle:
[1] V. Crepel and L. Fu, arXiv:2012.08528
[2] V. Crepel and L. Fu, arXiv:2103.12060
[3] K. Slagle and L. Fu, Phys. Rev. B 102, 235423 (2020)



3-Particle Mechanism for Superconductivity

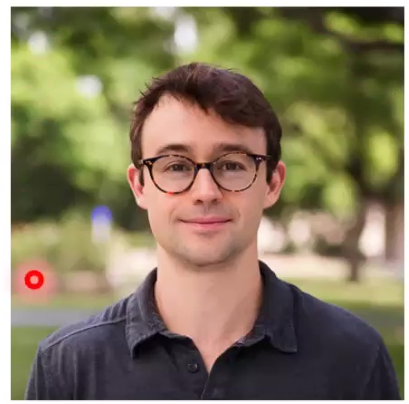
Liang Fu

Valentin Crepal
(MIT)

arXiv:2012.08528

arXiv:2103.12060

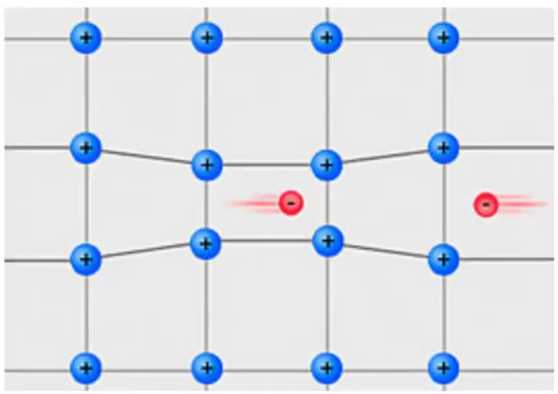
Kevin Slagle
(Caltech)

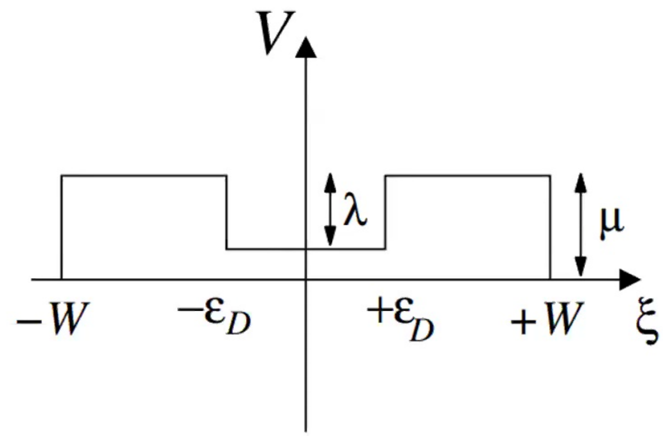


PRB 102, 235423 (2020)

Bardeen-Cooper-Schrieffer Theory

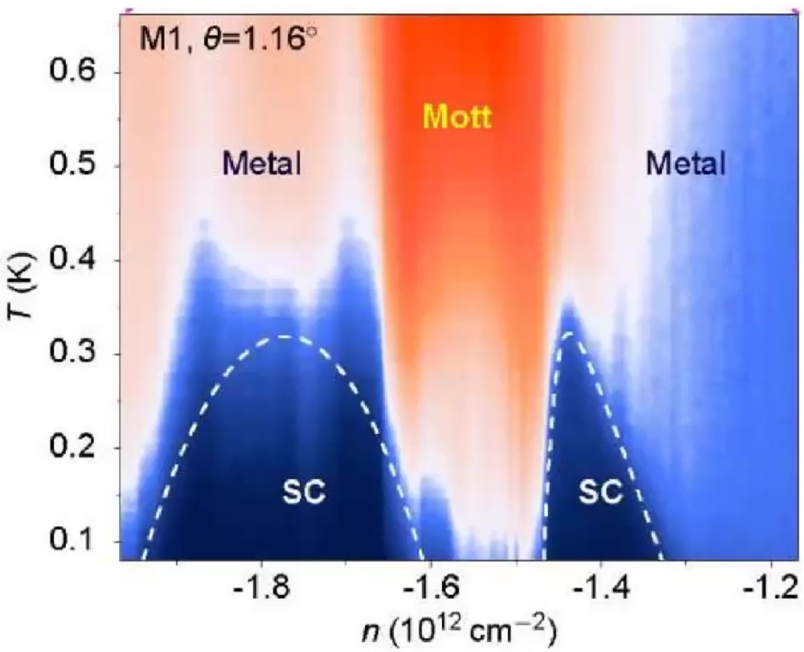
- Retarded attraction from electron-phonon interaction
- Downward renormalization of Coulomb repulsion



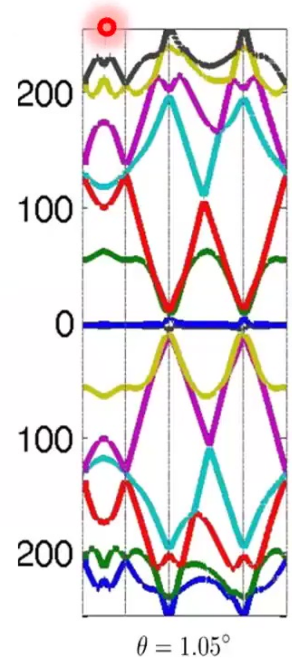


Retardation condition: Fermi energy >> Debye energy

Superconductivity in Narrow Bands



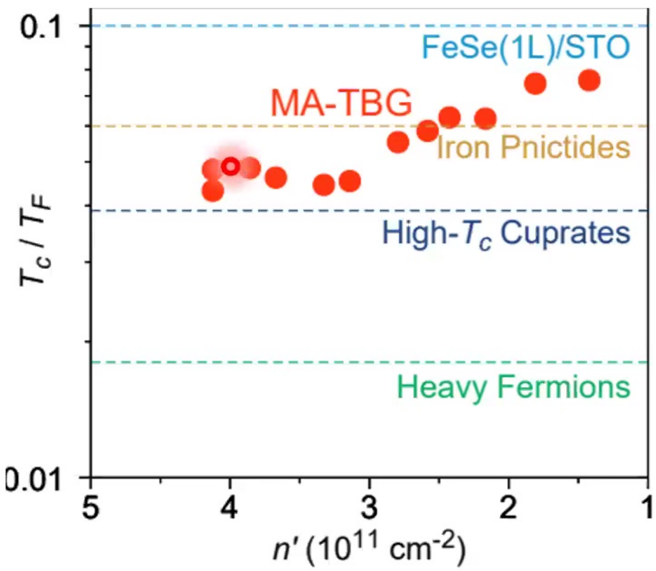
Cao et al, Nature (2018)



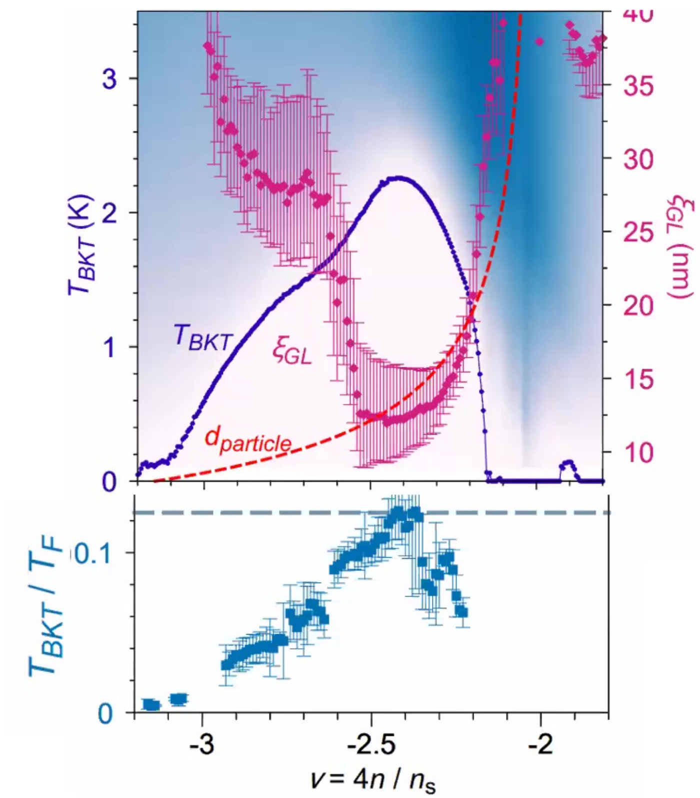
Bistrizer & MacDonald (2011)

Search for electronic mechanism of SC

Strong-Coupling SC with large T_c/T_F

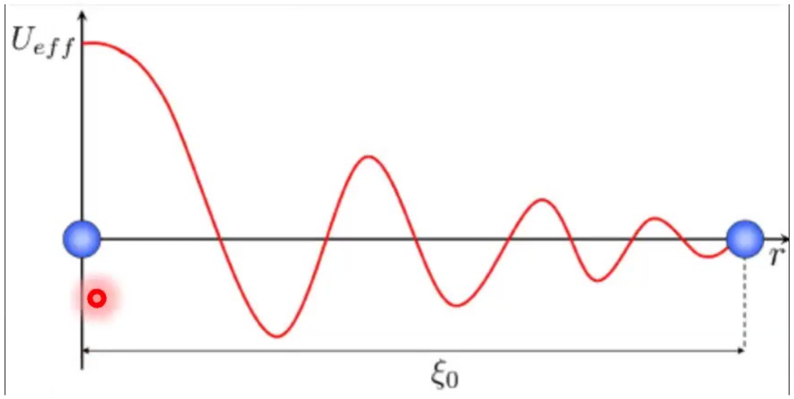


Cao et al, Nature (2018)



Park et al, Nature (2021)

Kohn-Luttinger Mechanism



Chubukov, Raghu, Kivelson, Scalapino, Guinea ...

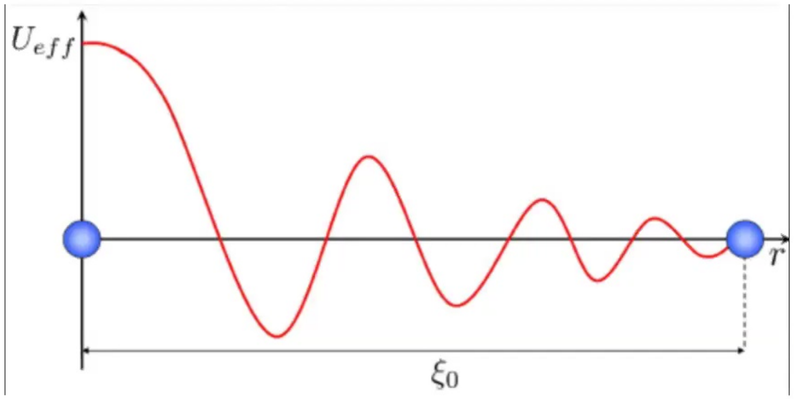
- attraction from polarization of Fermi liquid (*many-body* effect)
- asymptotically exact in *weakly interacting* limit $U \ll W$
- T_C is exponentially small

$$T_C \sim \exp\left(-\frac{1}{\rho U_{\text{eff}}}\right), \qquad U_{eff} \propto \frac{U^2}{W^2}$$

Challenge of **Strong-Coupling** SC

- lack of analytically controlled method
- abundance of competing states
- exponentially hard for numerical simulation

Kohn-Luttinger Mechanism



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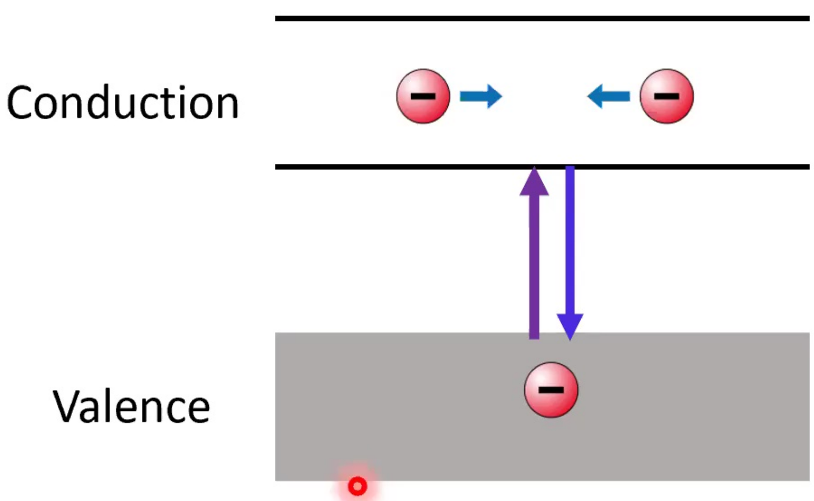
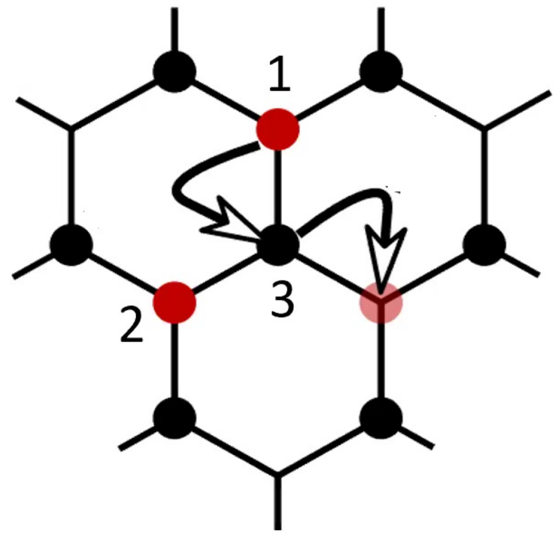
3-Particle Mechanism for SC

Crepel & LF, arXiv:2012.0852



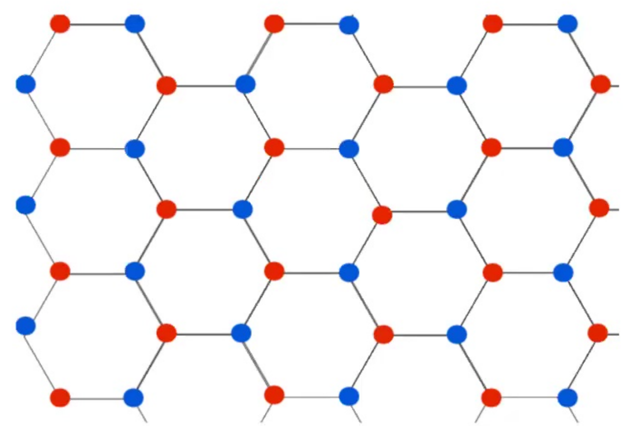


Controlled theory of SC from electron repulsion based on **strong-coupling** expansion in **kinetic term**

Our Model

Spin-polarized fermions on honeycomb lattice with nearest neighbor repulsion and staggered potential

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_t,$$
$$\mathcal{H}_0 = V \sum_{\langle r, r' \rangle} n_r n_{r'} + \Delta \sum_{r \in B} n_r,$$
$$\mathcal{H}_t = -t \sum_{\langle r, r' \rangle} (c_r^\dagger c_{r'} + hc).$$



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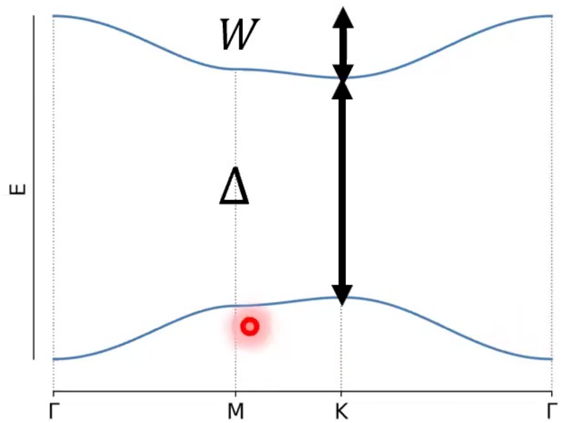
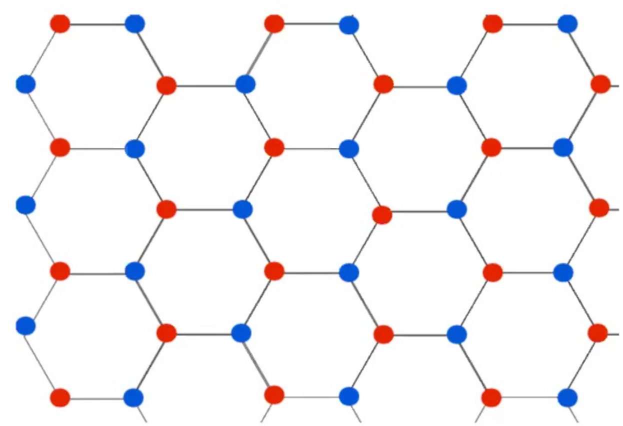
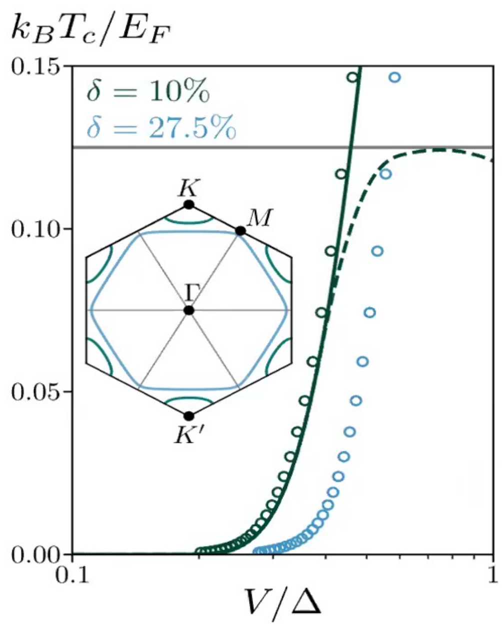




For small t, ground state at $n = 1$ is ionic band insulator

Strong-Coupling f-Wave SC upon Doping



At small (not too small) doping:

- $k_B T_c = 0.126\sqrt{\delta} \cdot W e^{-\frac{1}{2g_0}}$ accurate for $T_c \leq 0.1 E_F$

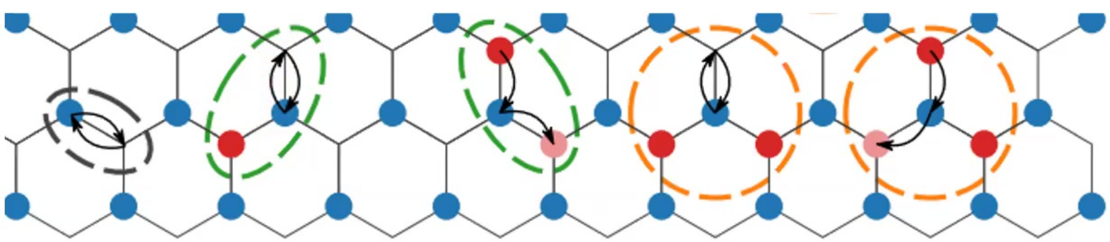
  with $W = \frac{9t^2}{\Delta + V}$, $g_0 = \frac{6V^2}{\pi\Delta(\Delta + 2V)}$ (**nonperturbative** in V)

- $\frac{\Delta}{k_B T_c} \approx 4.79$

Strong-Coupling Expansion

Starting point: interacting electrons in real space

- first-order process creates hole on A sites with high energy
- low-energy physics governed by second-order processes



Strong-Coupling Expansion in in Hopping $\boldsymbol{t}$

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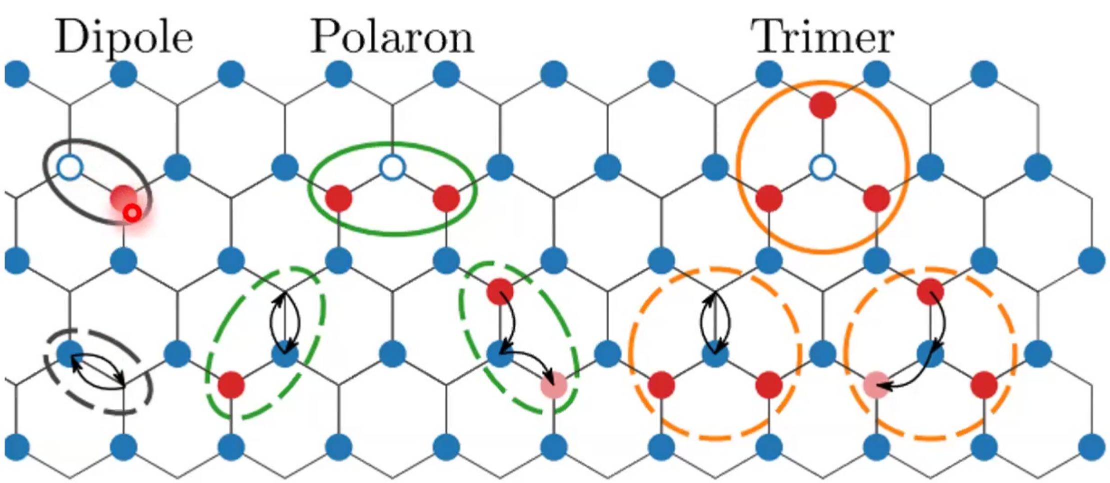
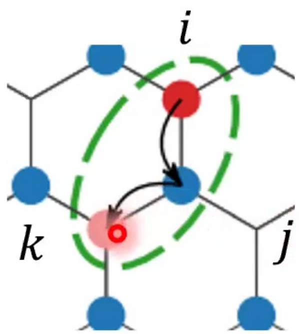


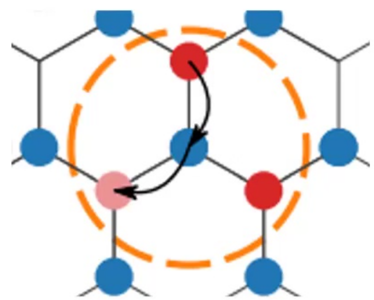
- Intermediate states involve dipoles, polarons and trimers

$$E_d = \Delta + 2V, \qquad E_p - E_f = \Delta + V, \qquad E_t - 2E_f = \Delta$$

3-Particle Process



$\delta E = \Delta + V$



$\delta E = \Delta$

Due to interaction V, the energy of intermediate state and the hopping amplitude of a doped electron from site $i \rightarrow k$ depends on occupation of adjacent site j.

$$t_f(f_i^\dagger f_j + hc) \qquad t_f = \frac{t^2}{\Delta + V},$$

$$\lambda(f_i^\dagger n_j f_k + P_{ijk}) \qquad \lambda = \frac{t^2}{\Delta} - \frac{t^2}{\Delta + V}$$

Effective Hamiltonian for Doped Fermions

from Schrieffer-Wolf transformation: $\mathcal{H}' = e^{iS}\mathcal{H}e^{-iS}$

$$\mathcal{H}' = \sum_{\langle i,j \rangle} t_f (f_i^\dagger f_j + hc) + V_f n_i n_j \; + \sum_{(ijk)\in\triangle} \lambda (f_i^\dagger n_j f_k + P_{ijk}) + U_3 n_i n_j n_k.$$

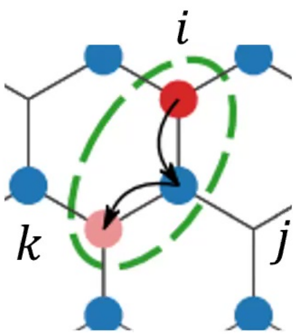
correlated hopping   3-body repulsion

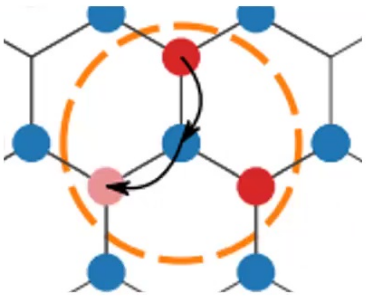
$$t_f = \frac{t^2}{\Delta + V}, \qquad V_f = -\frac{t^2}{\Delta} + \frac{4t^2}{\Delta + V} - \frac{3t^2}{\Delta + 2V},$$

$$\lambda = \frac{t^2}{\Delta} - \frac{t^2}{\Delta + V} \qquad U_3 = \frac{3t^2}{\Delta} - \frac{6t^2}{\Delta + V} + \frac{3t^2}{\Delta + 2V}.$$

- EXACT for any doping & interaction V in narrow band limit
- effective interaction is instantaneous
- longer-range interaction can be included straightforwardly

3-Particle Process





$\delta E = \Delta + V$ $\delta E = \Delta$

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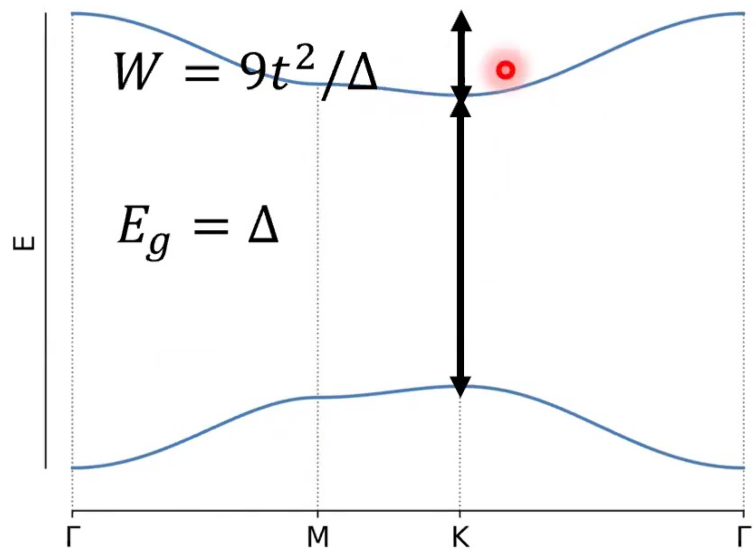
$$t_f(f_i^\dagger f_j + hc) \qquad t_f = \frac{t^2}{\Delta + V},$$

$$\lambda(f_i^\dagger n_j f_k + P_{ijk}) \qquad \lambda = \frac{t^2}{\Delta} - \frac{t^2}{\Delta + V}$$

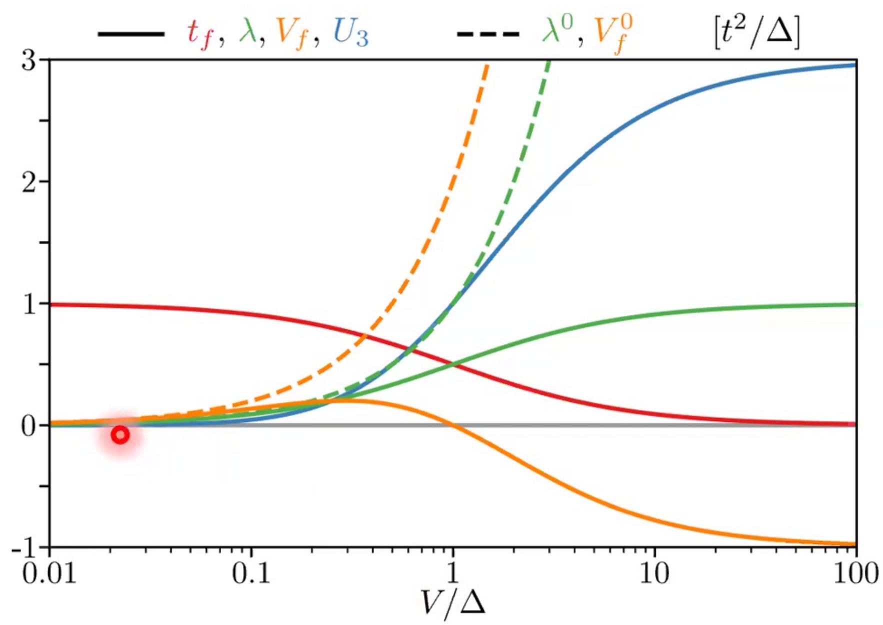
Weakly Interacting Limit $V \to 0$



Projecting bare interaction V directly into conduction band yields:

$$V_f^0 = 2\lambda^0 = \frac{2t^2}{\Delta^2} V$$

Interband Renormalization

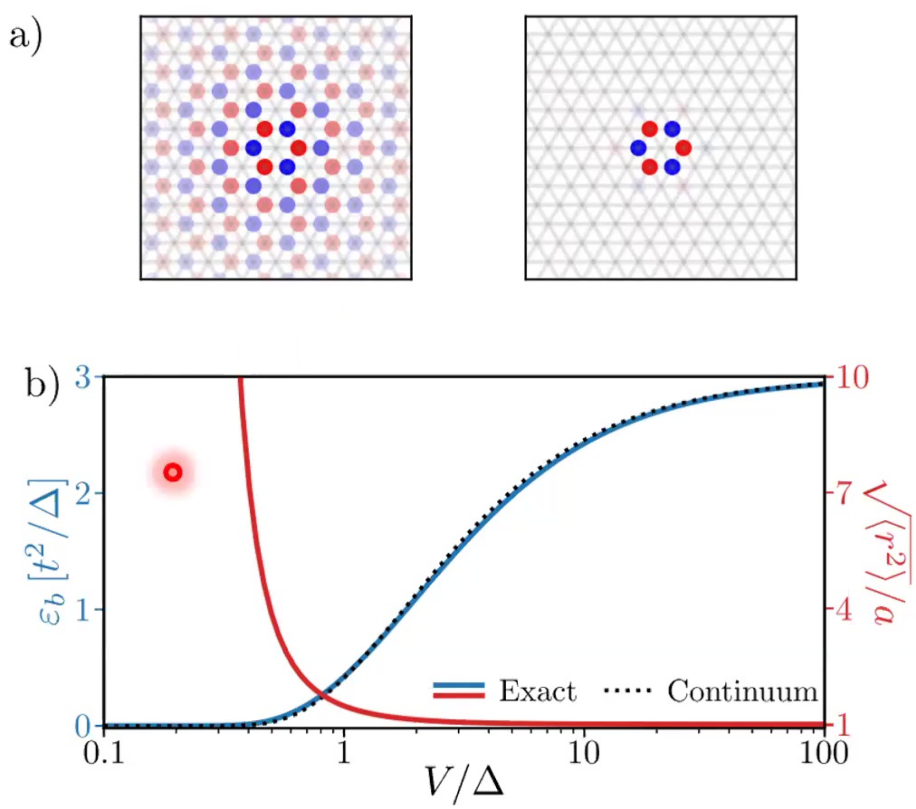


- Interaction is strongly renormalized by interband processes even for $V/\Delta = 0.1$.
- For $V < \Delta$, interactions between doped electrons are small compared to the bandwidth.

Two-Particle Bound State

from **exact** solution of lattice model H'

f-wave pairing



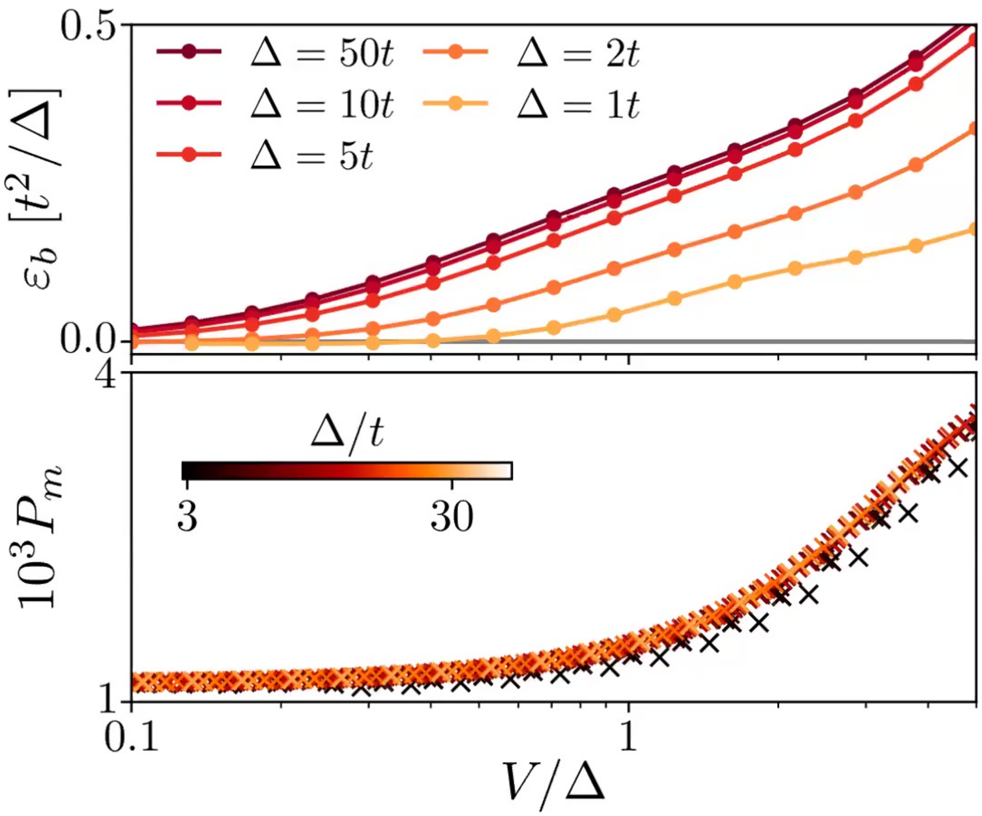
Binding energy
$\epsilon_b = 2E_e - E_{2e}$

Cooper pair size

Pairing from pure repulsion!

Exact Diagonalization for Full Model H

N=30 sites: $\epsilon_b = 2E\left(\frac{N}{2}+1\right) - E\left(\frac{N}{2}+2\right) - E\left(\frac{N}{2}\right)$



Continuum Theory at Low Density

$$\mathcal{H}' = \sum_{\langle i,j \rangle} t_f (f_i^\dagger f_j + hc) + V_f n_i n_j \; + \sum_{(ijk)\in\triangle} \lambda (f_i^\dagger n_j f_k + P_{ijk}) + U_3 n_i n_j n_k.$$

Low-energy modes around band bottom at $\pm K$

$$\widetilde{\mathcal{H}} = \int \mathrm{d}x \sum_{\tau=\pm} \psi_\tau^\dagger \left[\frac{-\nabla^2}{2m} \right] \psi_\tau + g \psi_+^\dagger \psi_+ \psi_-^\dagger \psi_-,$$

with $m = 2/(3t_f a^2), \quad g = 6a^2(V_f - 2\lambda) < 0.$

Two-valley Fermi liquid with attractive contact interaction:

- BCS-BEC crossover tuned by interaction and density
- s-wave valley-singlet = f-wave pairing on the lattice

Continuum Theory at Low Density

Binding energy: $$\frac{\varepsilon_b}{\varepsilon_{\text{uv}}} = \left[e^{1/g_0} - 1\right]^{-1} \quad g_0 = \frac{9}{\pi}\frac{2\lambda - V_f}{W} = \frac{6}{\pi}\frac{V^2}{\Delta(\Delta + 2V)}$$

UV energy cutoff is fixed by exact lattice calculation at $V = \infty$

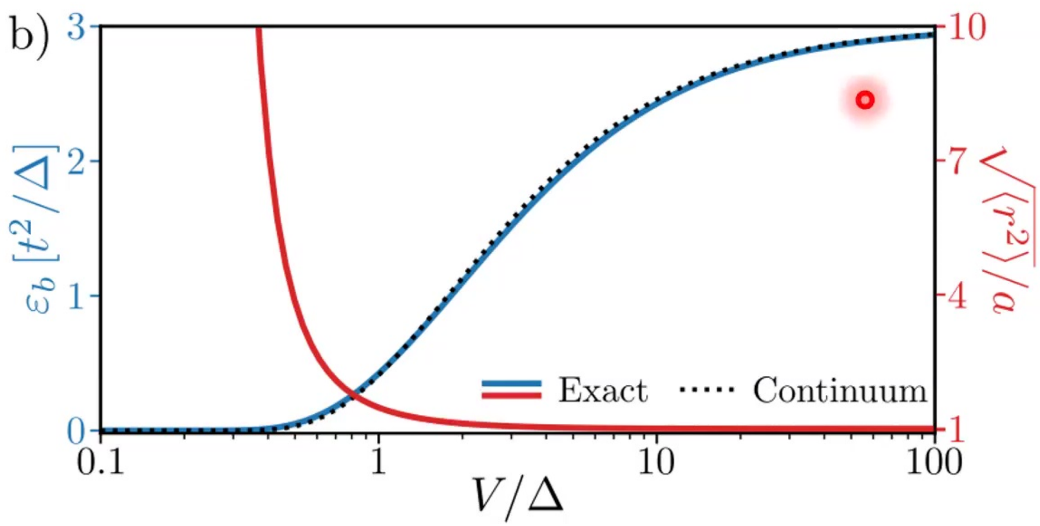
$$\varepsilon_{\text{uv}} = \pi W/9$$

g_0: dimensionless coupling constant

- at small V, $g_0 \propto V^2$ (exciton-mediated pairing)
- non-perturbative in V, exact in narrow band $t \ll \Delta$

Continuum Theory at Low Density

Binding energy: $$\frac{\varepsilon_b}{\varepsilon_{\mathrm{uv}}} = \left[e^{1/g_0} - 1\right]^{-1}$$



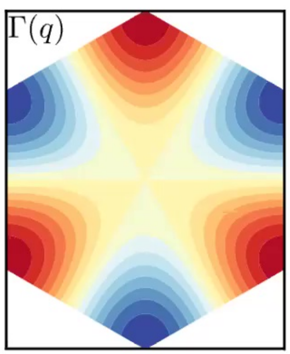
f-wave Superconductivity at Finite Density

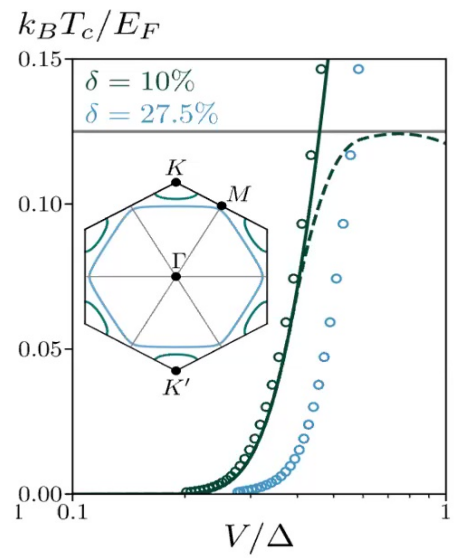
$$\mathcal{H}' = \sum_{\langle i,j \rangle} t_f (f_i^\dagger f_j + hc) + V_f n_i n_j + \sum_{(ijk)\in\triangle} \lambda (f_i^\dagger n_j f_k + P_{ijk}) + U_3 n_i n_j n_k.$$

Pairing interaction: $\Gamma = 2\lambda - V_f - \left(\langle f_i^+ f_j \rangle + \delta\right) U_3$

(without interband renormalization Γ=0)

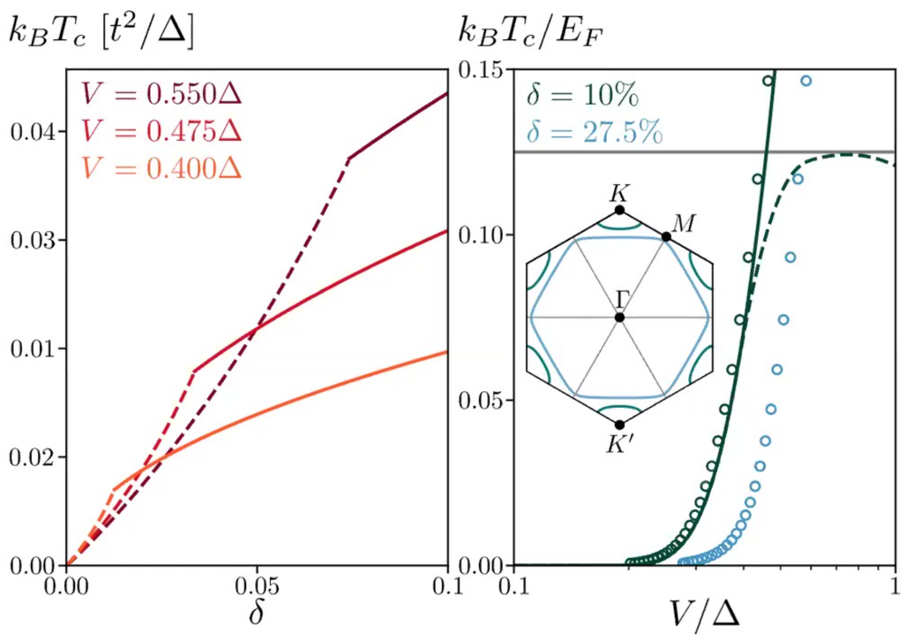
Gap function





full gap at $\delta < \frac{1}{4}$; point nodes at $\delta > \frac{1}{4}$

Strong-Coupling Superconductivity at Low Density



$$k_B T_c = e^{\gamma - 1}\sqrt{2E_F\varepsilon_b}/\pi \ = e^{\gamma-1}\sqrt{\frac{2E_F W}{9\pi}}e^{-1/(2g_0)}$$

shown to be accurate for $T_c \leq 0.1\ T_F$ by sign-problem-free QMC for attractive Fermi liquid (Shi, Chiesa & Zhang, PRA 2015)

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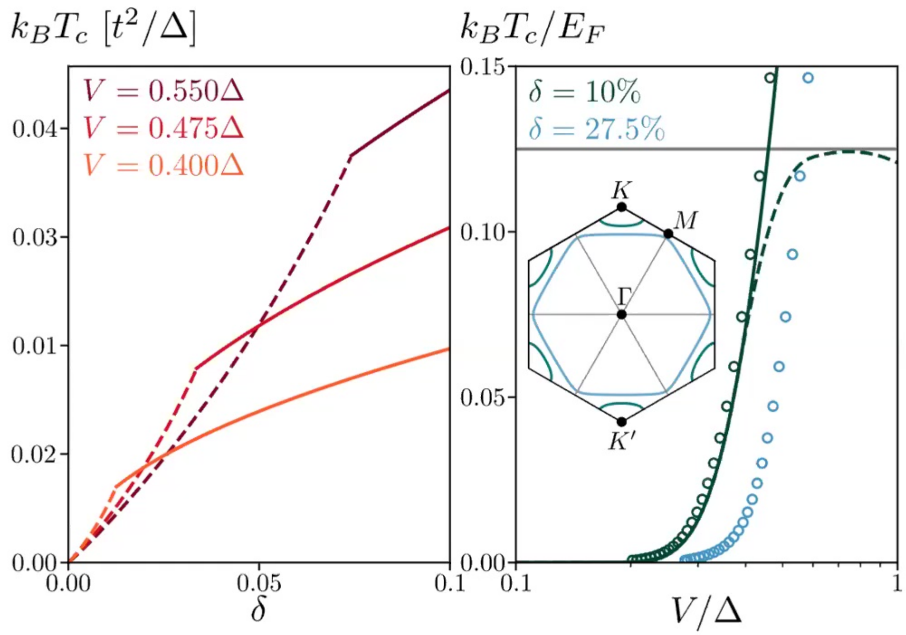
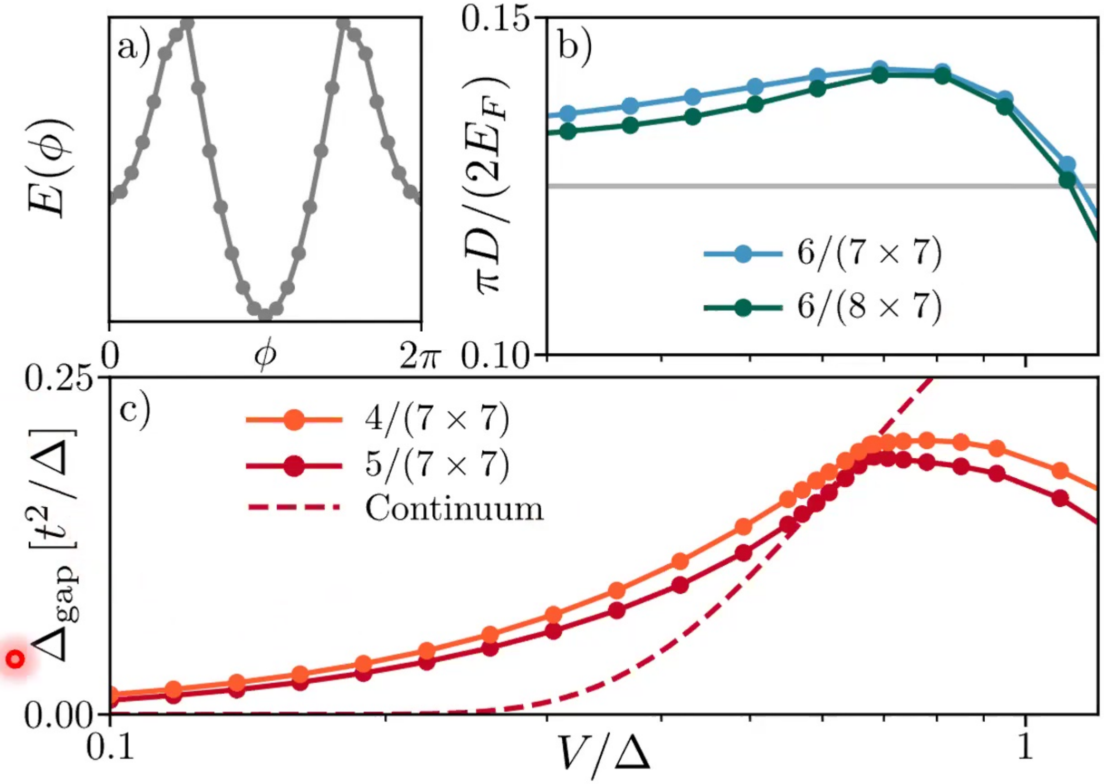


$\Delta_{\text{gap}}/k_BT_c = \pi e^{1-\gamma} \simeq 4.796,$ compared to 1.764 in BCS theory with Debye energy cutoff

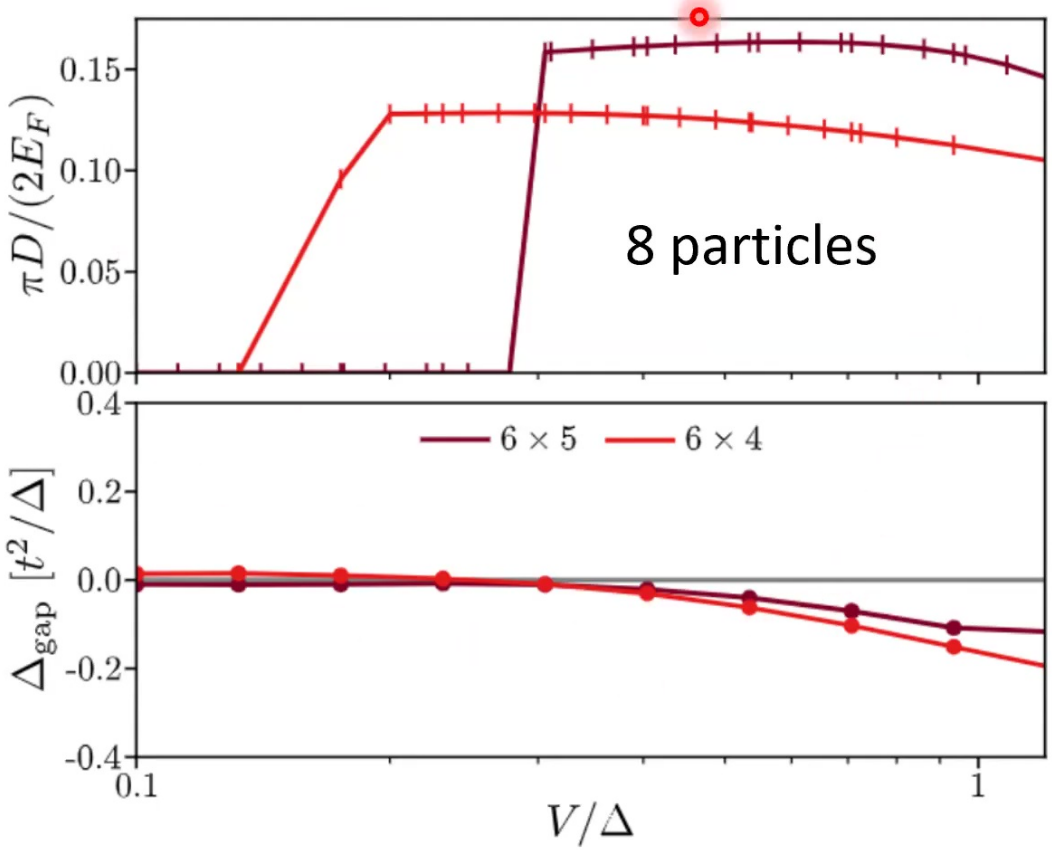
Exact Diagonalization



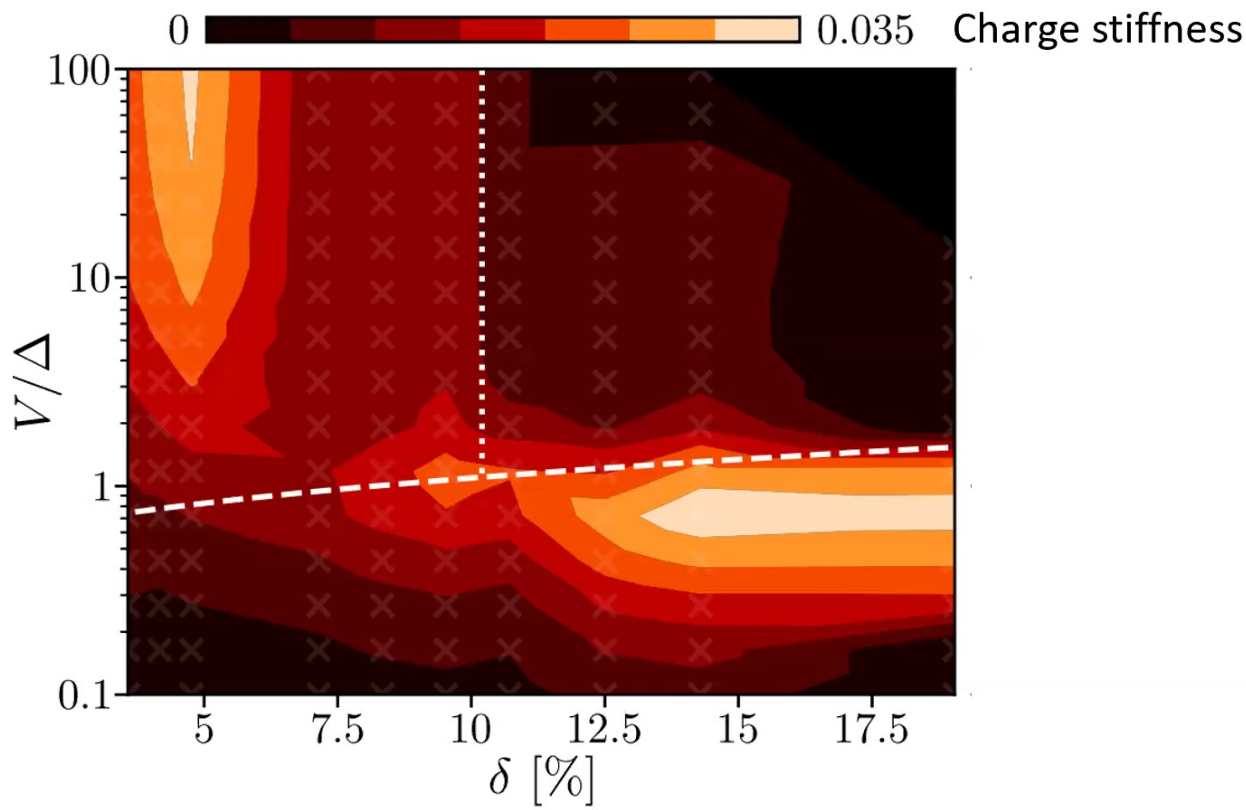
Charge stiffness : $D = \frac{1}{16\pi^2}\,\frac{L_1}{L_2}\,\frac{\partial^2 E(N,\phi)}{\partial\phi^2}\Big|_{\phi=0}$

Pairing gap : $\Delta_{\rm gap} = \frac{(-1)^N}{2}\left[E(N+1)+E(N-1)-2E(N)\right]$

Nodal Superconductivity



Phase Separation at $V \gg \Delta$

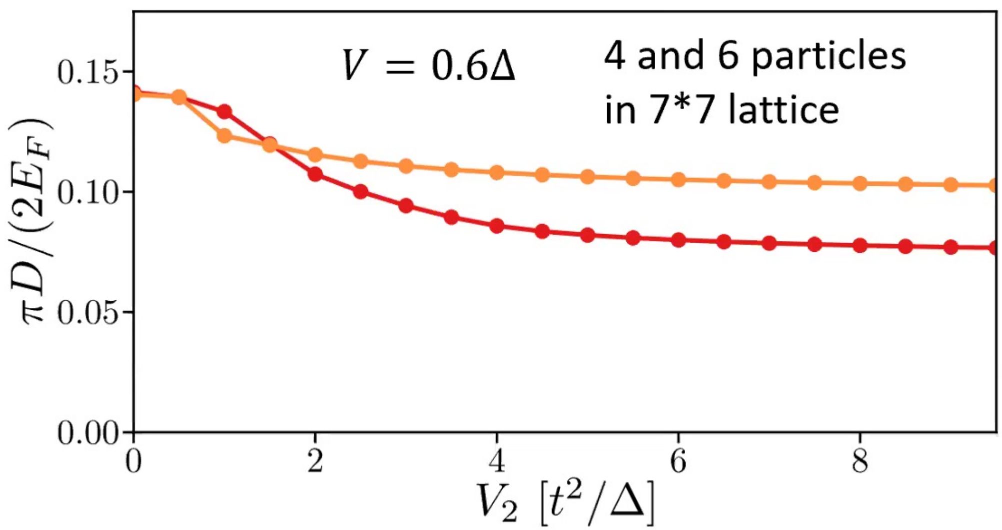


Possible competing states at commensurate doping and large V/Δ

Longer-Range Interaction

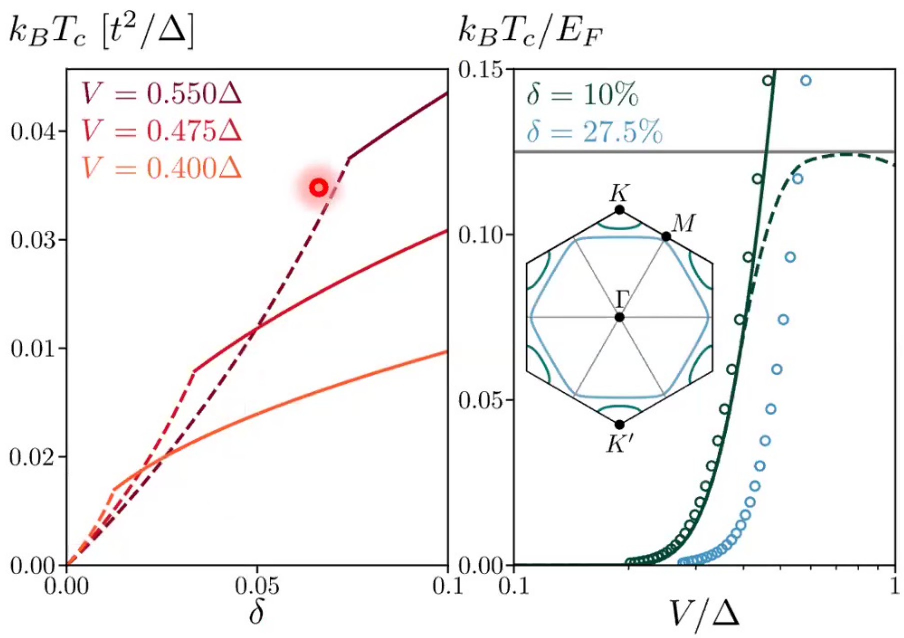
$$\mathcal{H}' = \sum_{\langle i,j \rangle} t_f(f_i^\dagger f_j + hc) + V_f n_i n_j \; + \sum_{(ijk)\in\triangle} \lambda(f_i^\dagger n_j f_k + P_{ijk}) + U_3 n_i n_j n_k .$$

For $V_2 \ll \Delta$, $V_f' = V_2 + V_f$.



SC at finite doping is remarkably robust against long-range interaction.

Strong-Coupling Superconductivity at Low Density



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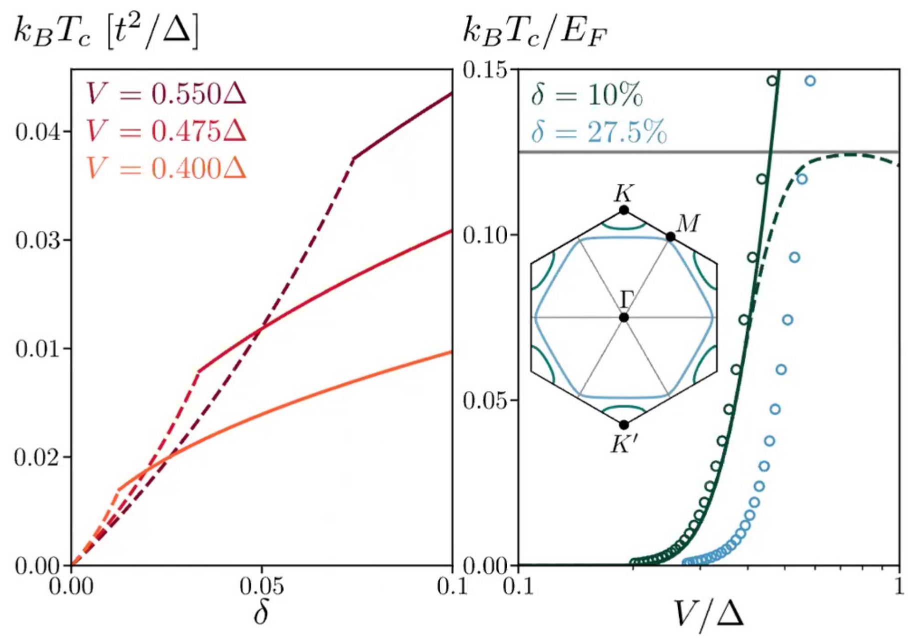

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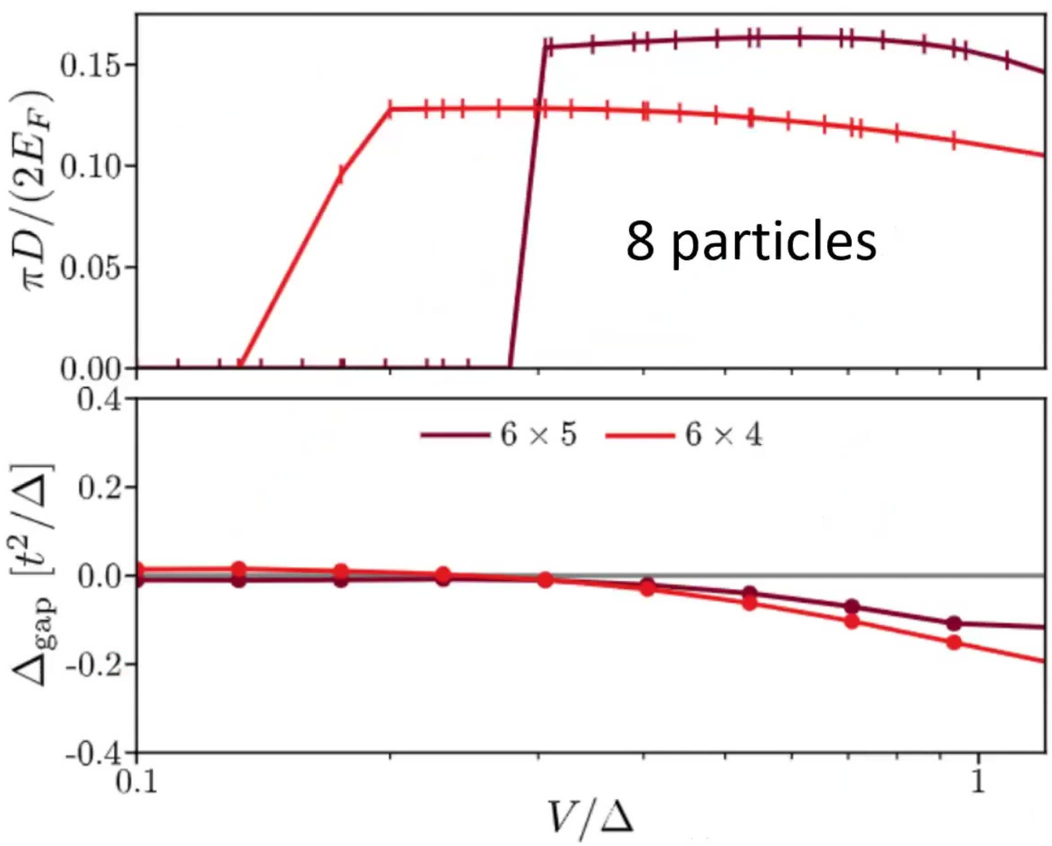
Nodal Superconductivity



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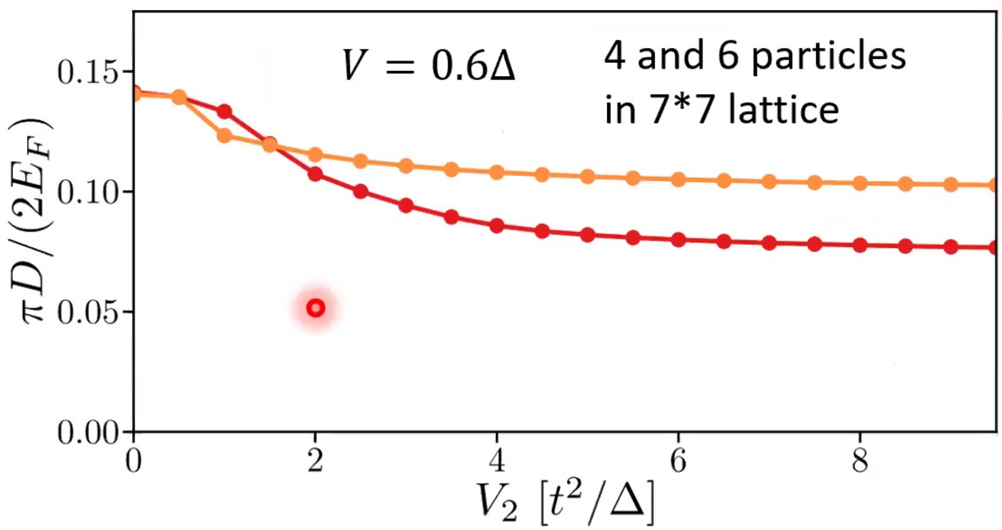
For $V_2 \ll \Delta$, $\quad V_f' = V_2 + V_f$.



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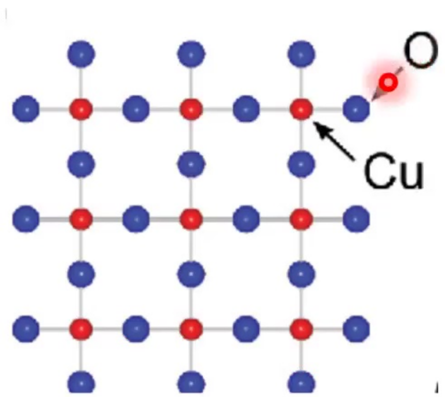
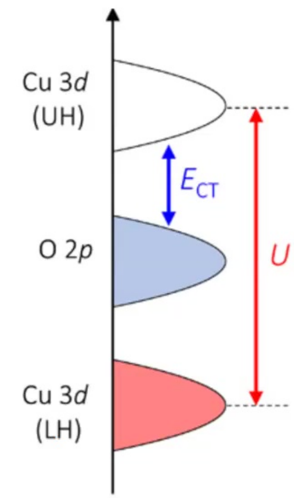
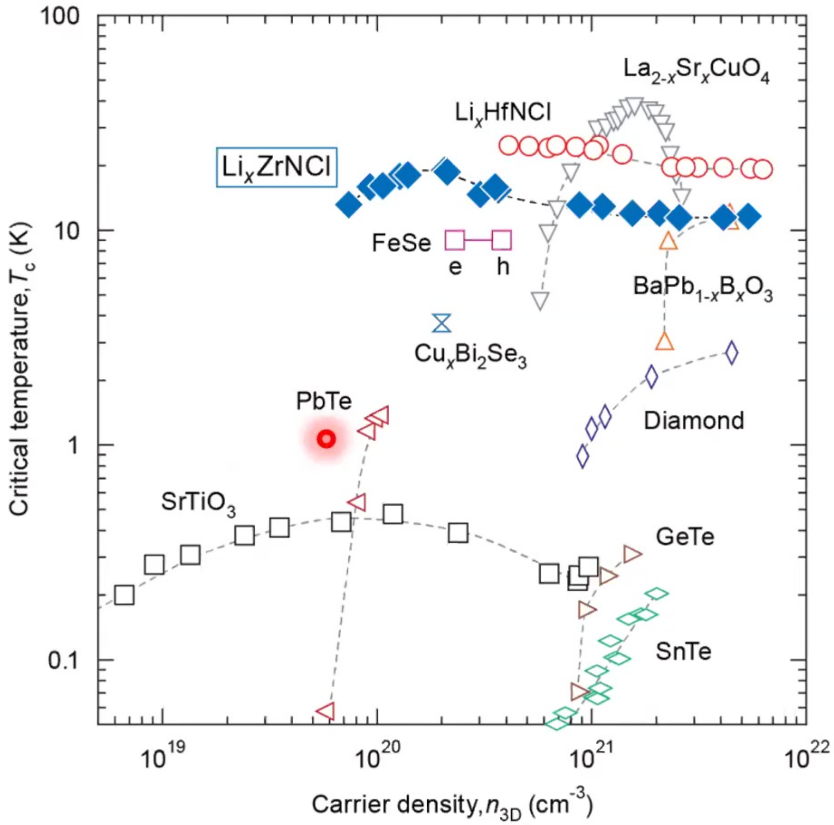
Spin-1/2 Multiband Systems





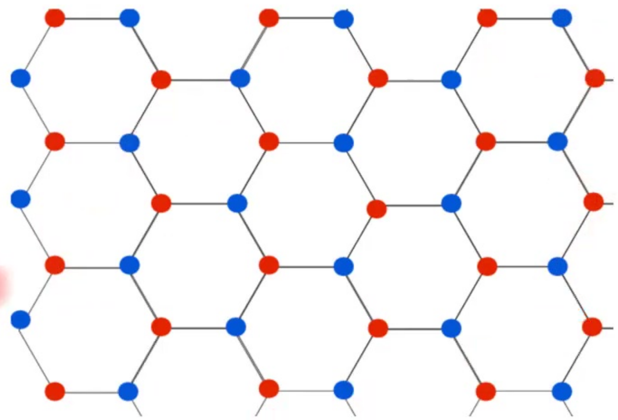
SC from doping a Mott/charge-transfer insulator

SC from Doping Band Insulators



Iwasa et al, arXiv (2020)

Our Model 2.0



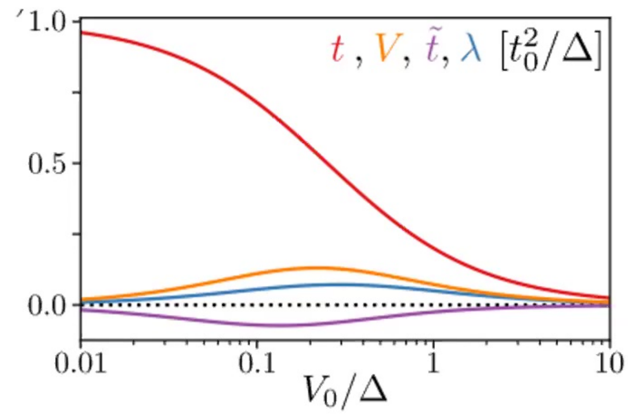
$$\mathcal{H} = -t_0 \sum_{\langle r,r' \rangle} (c_r^\dagger c_{r'} + c_{r'}^\dagger c_r) + \Delta_0 \sum_{r \in B} n_r \qquad (1)$$

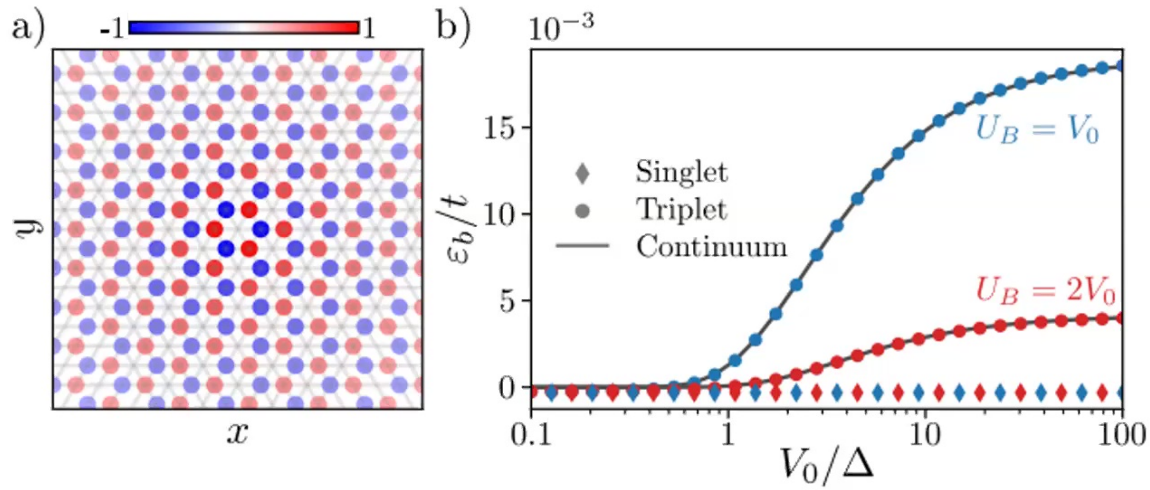
$$+ U_A \sum_{r \in A} n_{r\uparrow} n_{r\downarrow} + U_B \sum_{r \in B} n_{r\uparrow} n_{r\downarrow} + V_0 \sum_{\langle r,r' \rangle} n_r n_{r'},$$

Crepel & LF, arXiv:2103.12060

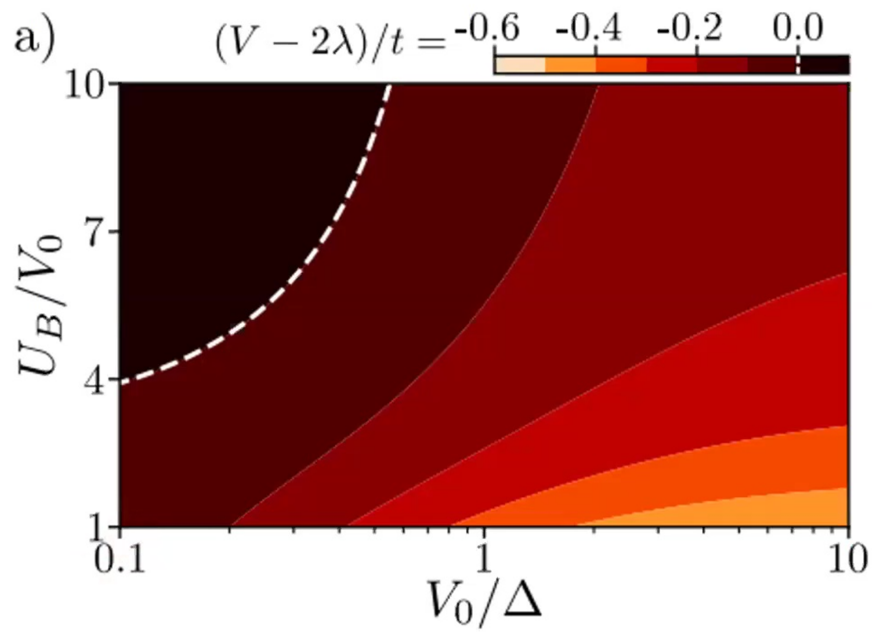
f-Wave Spin-Triplet & Valley-Singlet Pairing

$$
\begin{aligned}
\mathcal{H}_f = t \sum_{\langle i,j \rangle,\sigma} (f^\dagger_{j,\sigma} f_{i,\sigma} + hc) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j \\
+ \frac{\tilde{t}}{2} \sum_{\langle i,j \rangle,\sigma} (f^\dagger_{j,\sigma} f_{i,\sigma} + hc)(n_i + n_j) \\
+ \lambda \sum_{ijk \in \triangle,\sigma} \left[f^\dagger_{j,\sigma} n_k f_{i,\sigma} + P_{ijk} \right] \qquad (2)
\end{aligned}
$$





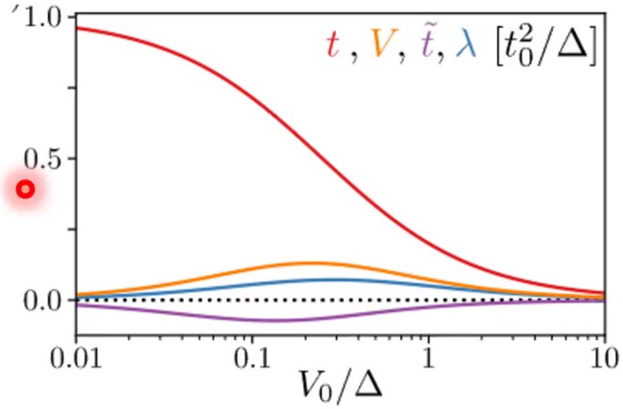
Two-Particle Bound State

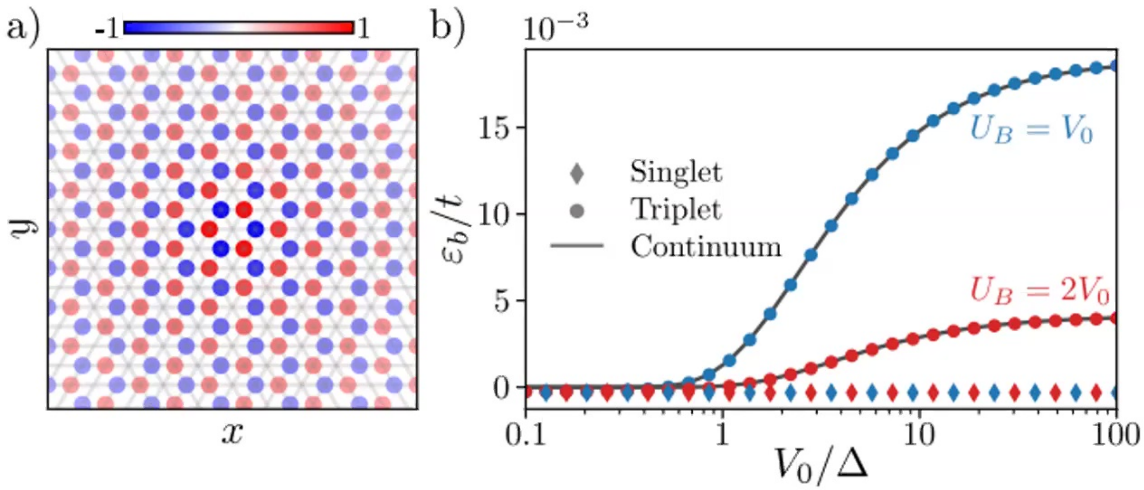


- At large U_B/V_0, pairing requires a minimum interaction V_0.
- Bound state remains with longer-range interaction $V_2 < 2\lambda - V$.

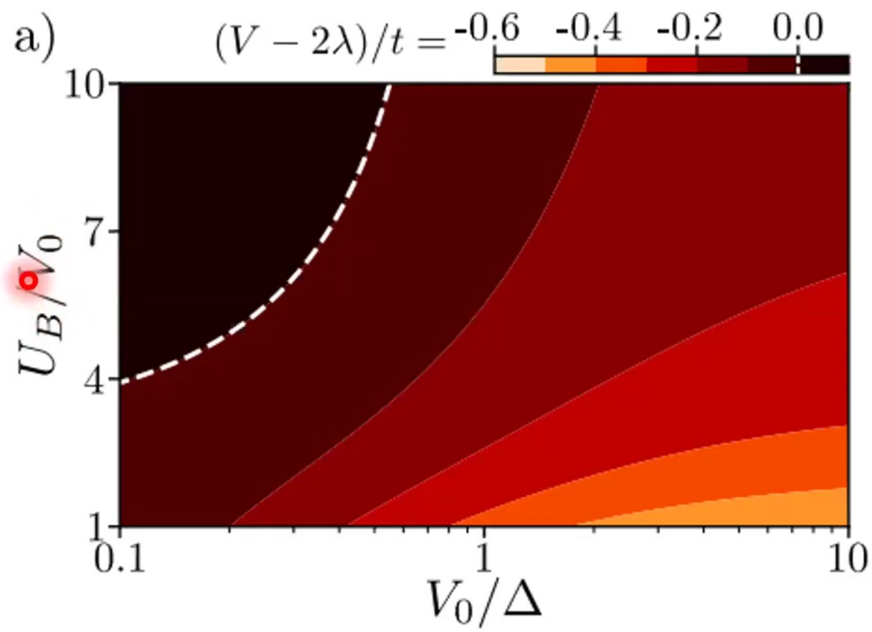
f-Wave Spin-Triplet & Valley-Singlet Pairing

$$\mathcal{H}_f = t \sum_{\langle i,j \rangle, \sigma} (f^\dagger_{j,\sigma} f_{i,\sigma} + hc) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j + \frac{\tilde{t}}{2} \sum_{\langle i,j \rangle, \sigma} (f^\dagger_{j,\sigma} f_{i,\sigma} + hc)(n_i + n_j) + \lambda \sum_{ijk \in \triangle, \sigma} \left[f^\dagger_{j,\sigma} n_k f_{i,\sigma} + P_{ijk} \right] \quad (2)$$





Two-Particle Bound State



- At large U_B/V_0, pairing requires a minimum interaction V_0.
- Bound state remains with longer-range interaction $V_2 < 2\lambda - V$.

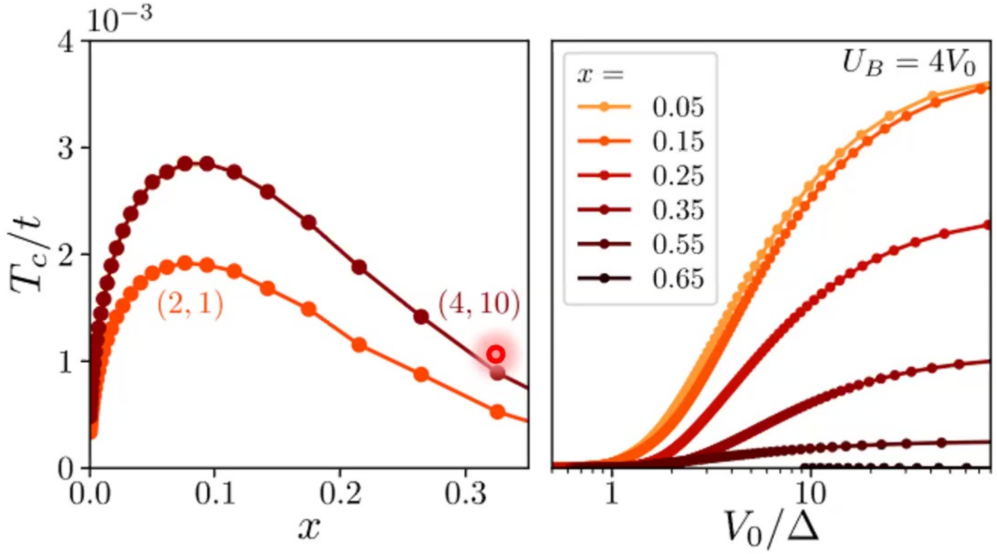
Two-Valley Fermi Liquid at Low Density

$$\tilde{H}_0 = \int \mathrm{d}x \sum_{\sigma\tau} \psi^\dagger_{\sigma\tau} \left[\frac{-\nabla^2}{2m}\right] \psi_{\sigma\tau}$$

$$\tilde{\mathcal{H}}_i = \int \mathrm{d}x \; g_0(\rho_{K\uparrow}\rho_{K\downarrow} + \rho_{K'\uparrow}\rho_{K'\downarrow}) + g_1 \rho_K \rho_{K'} + g_2 \mathbf{s}_K \cdot \mathbf{s}_{K'}$$

Virtual excitons produce strong ferromagnetic intervalley exchange interaction $|g_2| > 4g_1$ and lead to triplet pairing.

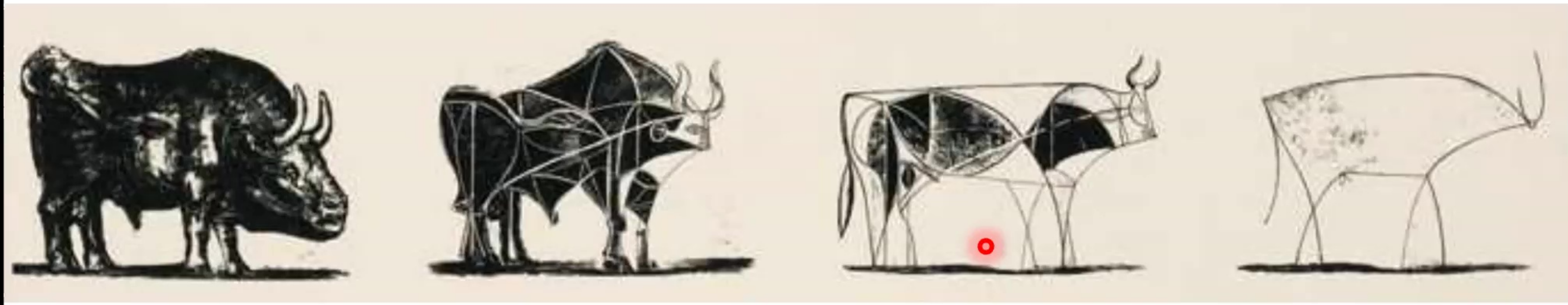
Critical Temperature



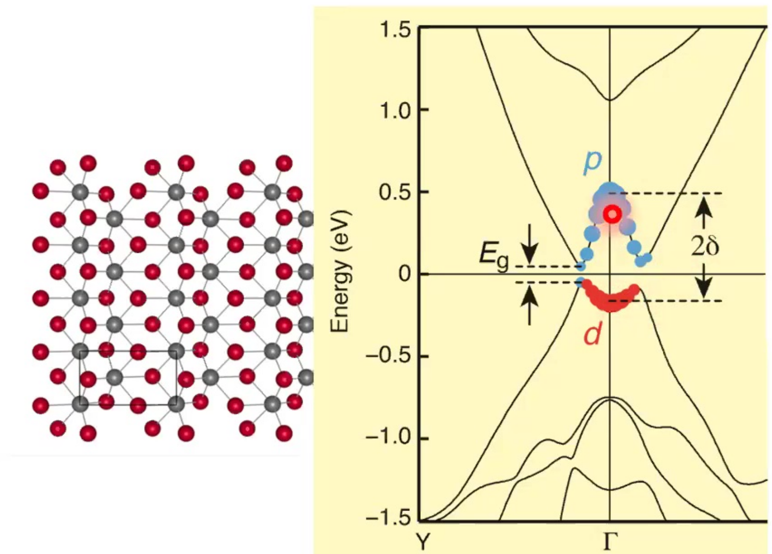
Doping band insulator *immediately* gives rise to *spin-triplet, valley-singlet* SC with full gap.

$$k_B T_c^{\mathrm{MF}} = \frac{e^{\gamma}}{\pi}\sqrt{\varepsilon_F \varepsilon_b} \propto \sqrt{xW}\exp\left(-\frac{4\pi}{m|g|}\right).$$

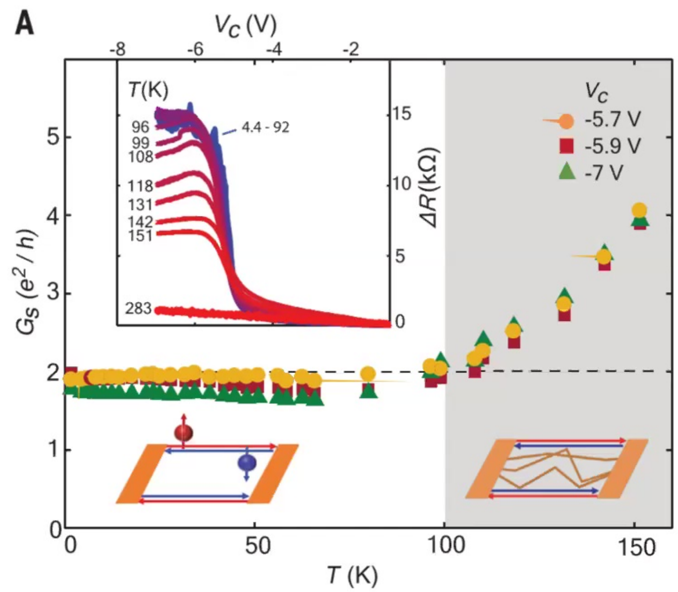
The Road to Simplicity



Monolayer WTe_2

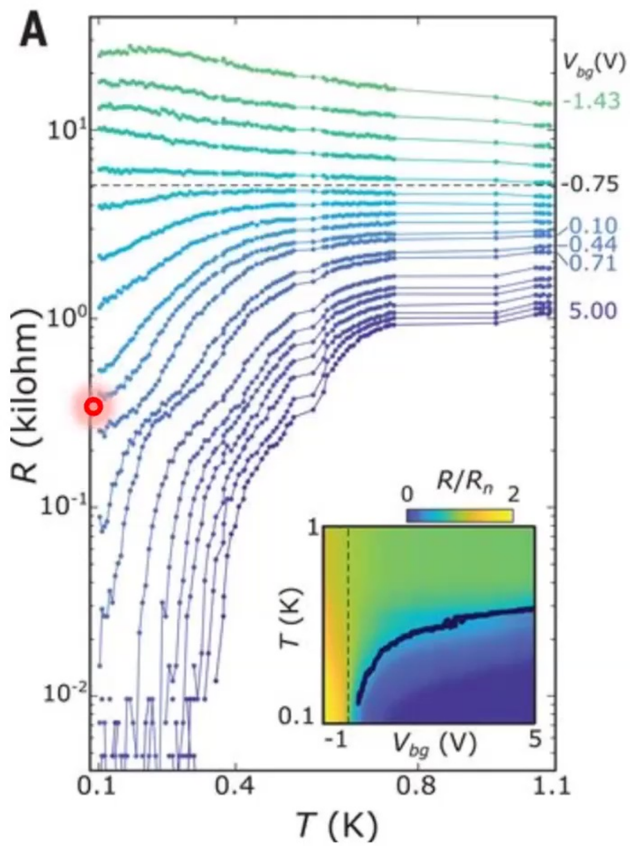


Qian, Liu, LF & Li, Science (2014)



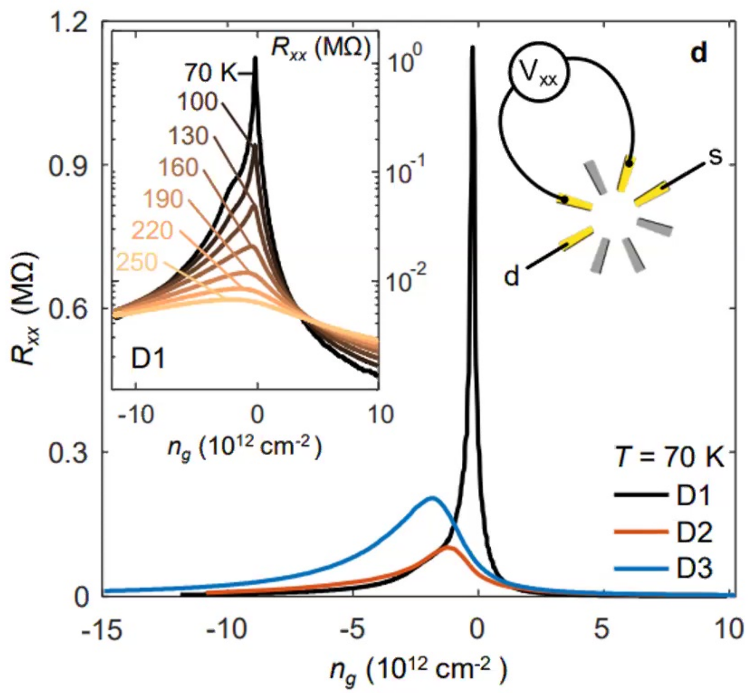
Wu, Fatemi et al, Science (2018)
Cobden et al, Nature Physics (2017)

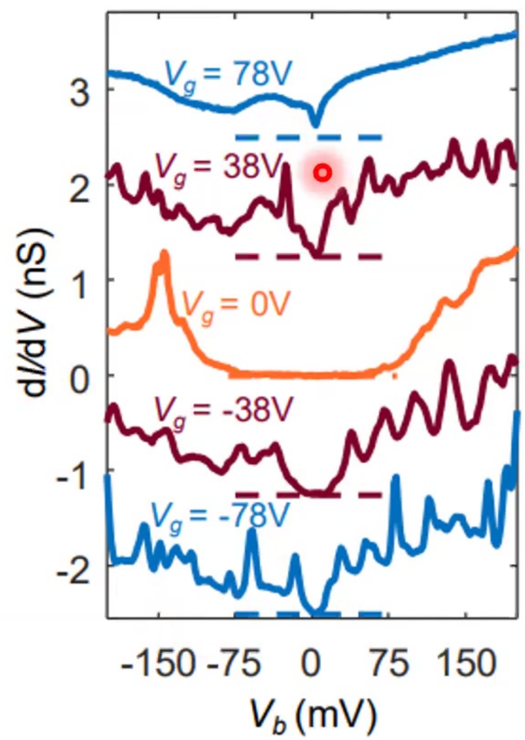
Superconductivity in Electron Doped WTe_2



Fatemi, Wu et al; Sajadi et al, Science (2018)

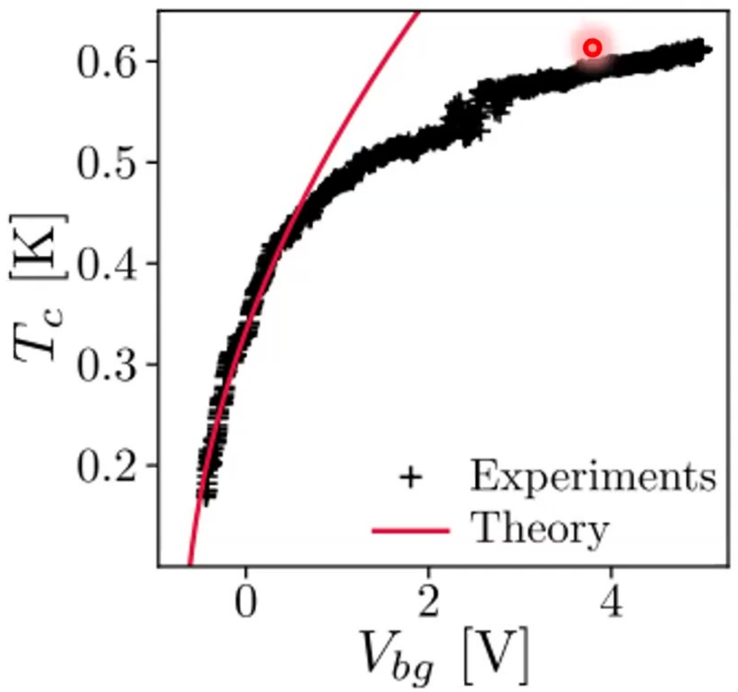
Strong Excitonic Effect in WTe_2





Wu & Yazdani, arXiv (2020)

Gating-Induced Insulator-SC Transition



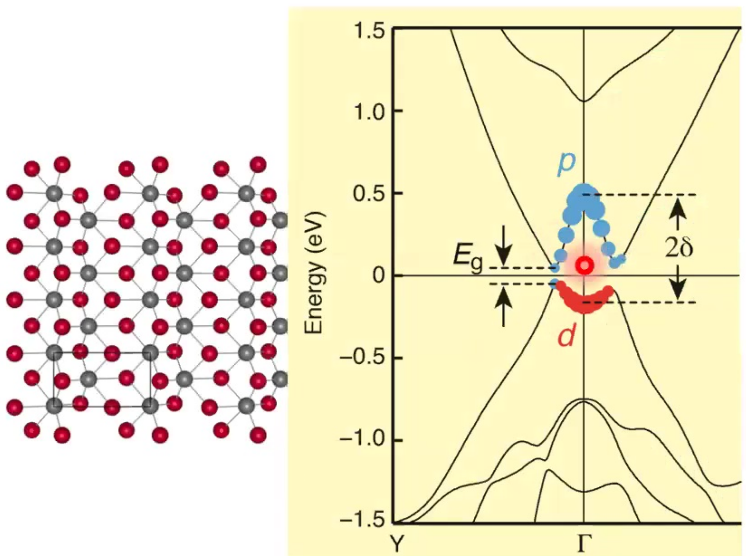
$T_c \propto \sqrt{x}$ at low doping

Prediction:

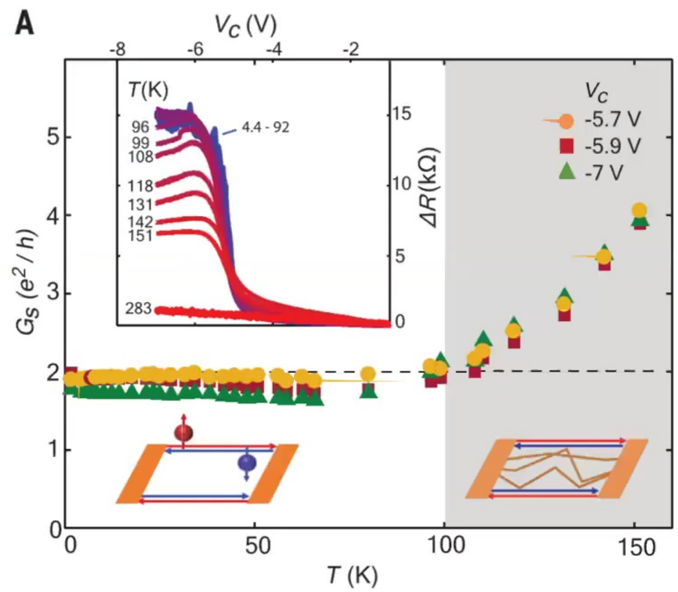
single-particle gap doesn't close;

$\frac{\Delta}{T_c}$ significantly larger than 1.75

Monolayer WTe_2

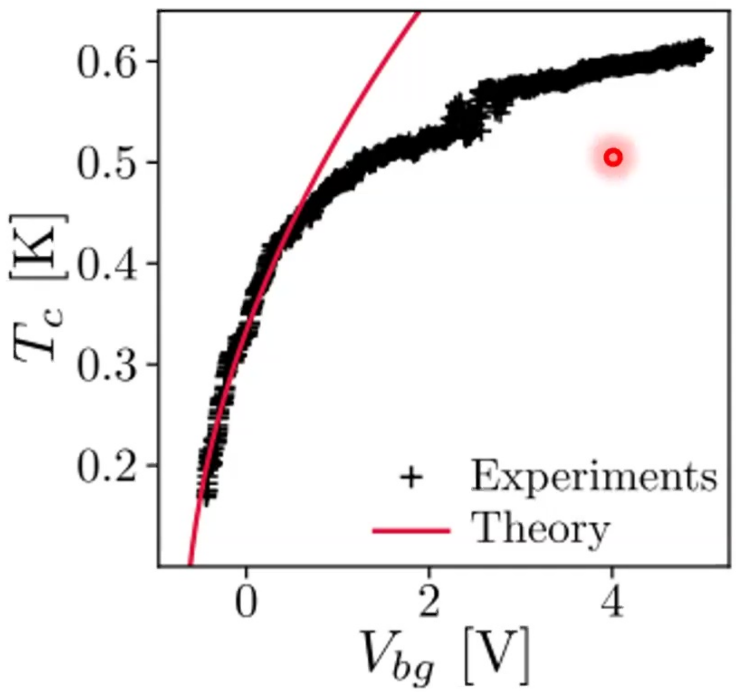


Qian, Liu, LF & Li, Science (2014)



Wu, Fatemi et al, Science (2018)
Cobden et al, Nature Physics (2017)

Gating-Induced Insulator-SC Transition



$T_c \propto \sqrt{x}$ at low doping

Prediction:

single-particle gap doesn't close;

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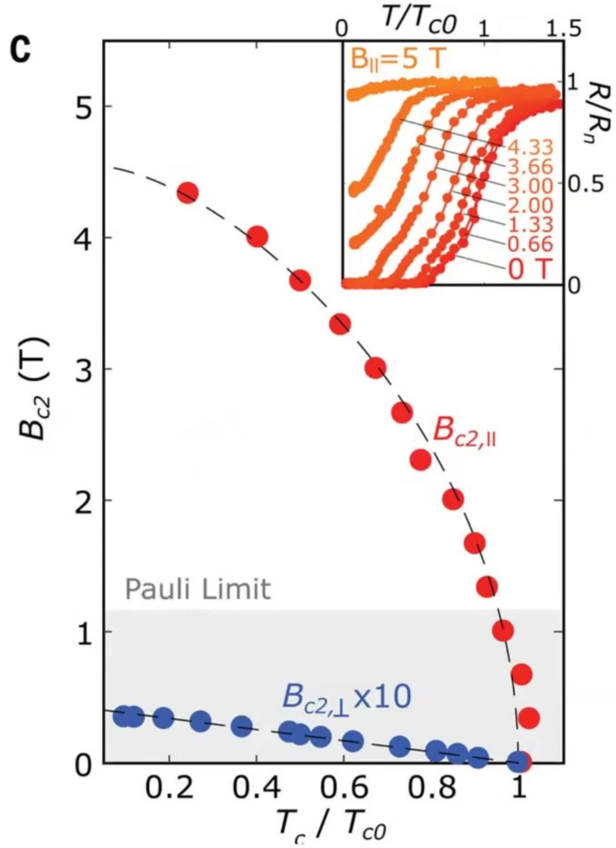
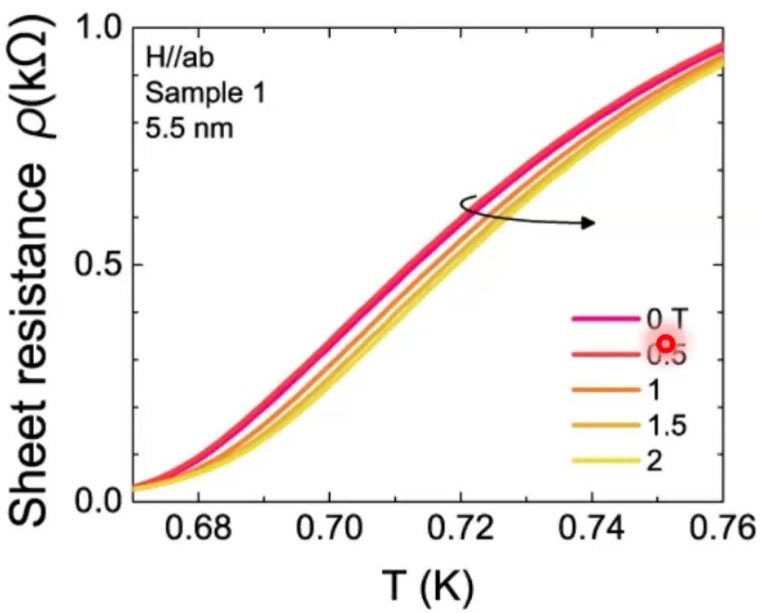
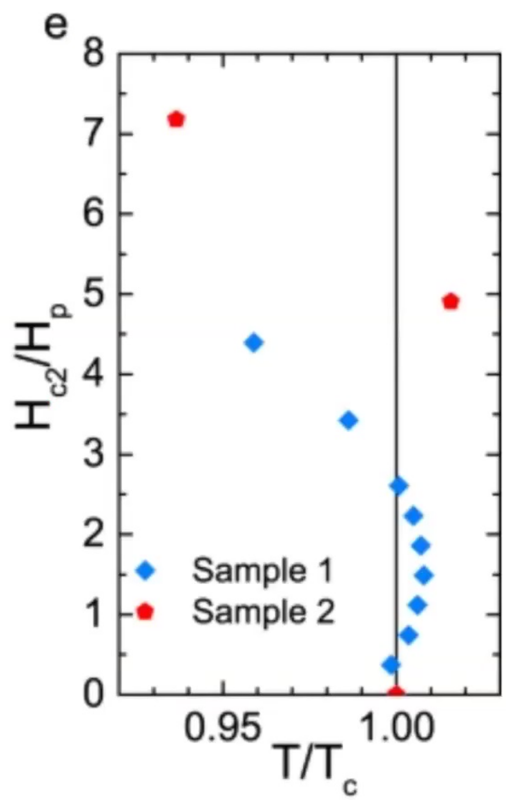
Large Violation of Pauli Limit



Magnetic Field Enhances Tc!





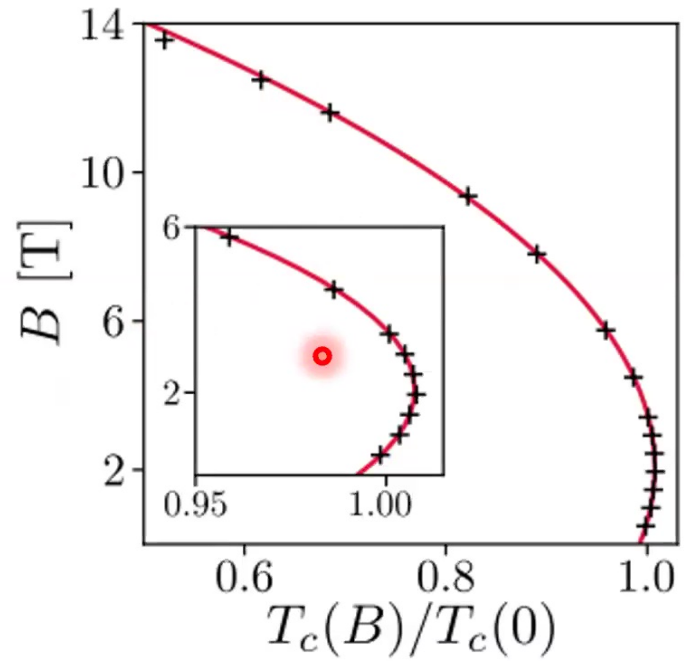
Lu Li, Sci. Rep. (2018)

Spin-Triplet SC in WTe_2

- Spin-triplet, valley-singlet pairing parameterized by d-vector
- Zeeman effect on triplet pairs

$$F = \alpha(\mathbf{d}\cdot\mathbf{d}^*)+\mu\mathbf{B}\cdot(i\mathbf{d}\times\mathbf{d}^*)+\eta|\mathbf{B}\cdot\mathbf{d}|^2+\chi B^2(\mathbf{d}\cdot\mathbf{d}^*),$$

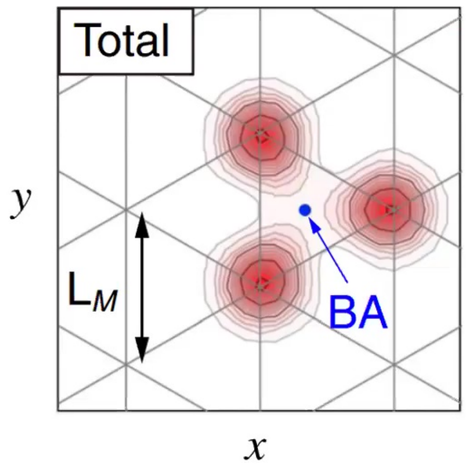
$$\Delta T_c^B = \mu B - \chi B^2$$



Crepel & LF, arXiv:2103.12060

Magic-Angle Graphene

Projecting Coulomb interaction directly into narrow band yields density repulsion & correlated hopping of comparable magnitude.



"The competition between the repulsion … and the assisted hopping term … can lead to many superconducting phases."
(Guinea & Walet, PNAS 2018)

Koshino et al; Kang & Vafek, PRX (2018)

Our theory suggests that virtual <u>interband processes</u> are essential for obtaining strong-coupling SC.

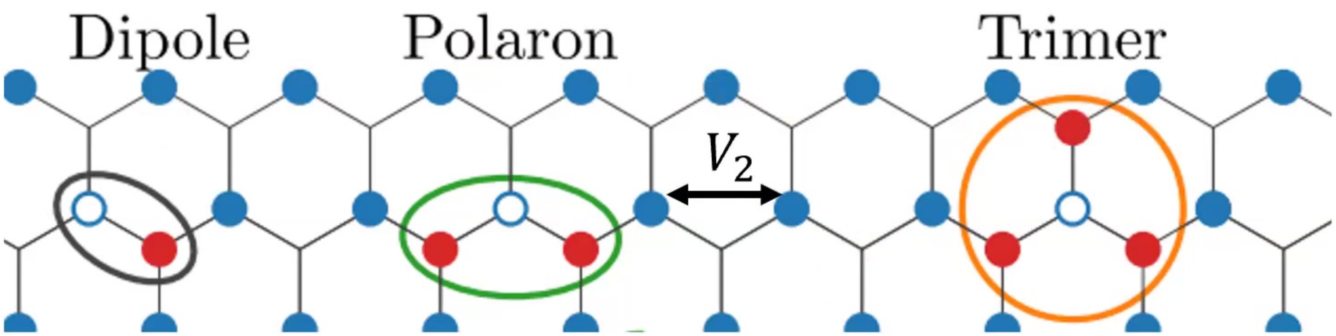
Theory of Strong-Coupling SC

- In narrow band systems, dynamics of nearby carriers on the lattice is correlated.
- Expansion in kinetic energy term provides a controlled theory of superconductivity from repulsive interaction.
- Correlated tunneling of 3 particles induces pairing within narrow band.
- T_c can reach as large as $0.1T_F$ when bare interaction and single-particle band gap are comparable.
- Unconventional pairing symmetry is easily obtained.
- Insulator-superconductor transition
- Possible realization in WTe_2 and graphene/TMD moire lattices

<u>Preformed</u> Trimers & Superconductivity

with Kevin Slagle
(Caltech)

Longer-Range Interaction

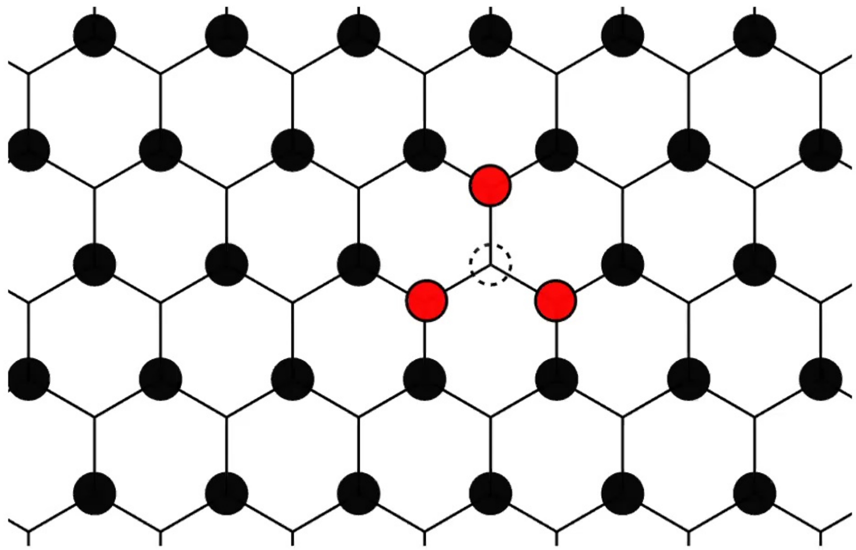


Dipole: $E_d = \Delta + 2V - 6V_2$

Polaron: $E_p - E_e = \Delta + V - 5V_2$

Trimer: $E_t - 2E_e = \Delta - 3V_2$

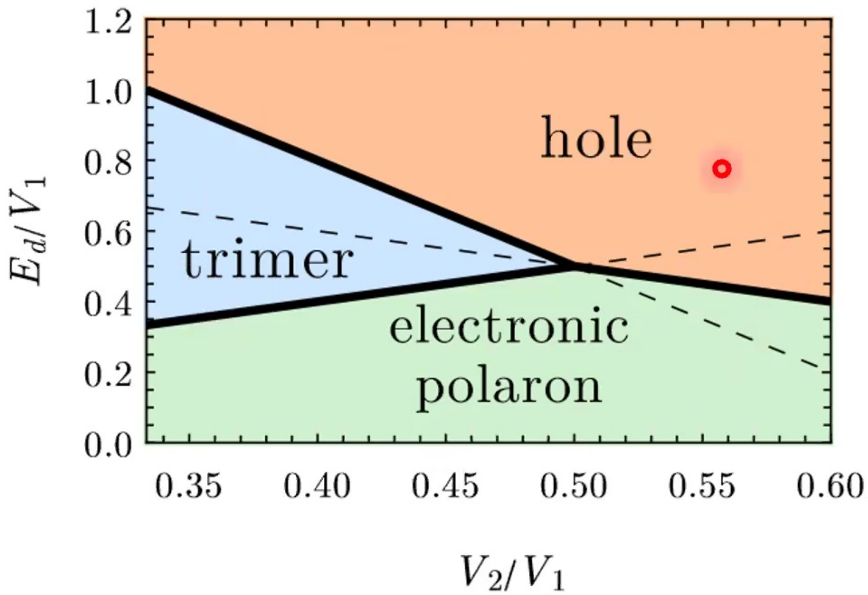
Less Repulsion is Attraction



When $E_t - 2E_1 = \Delta - 3V_2 + \cdots$ is negative,
trimer costs less energy than two separate electrons.

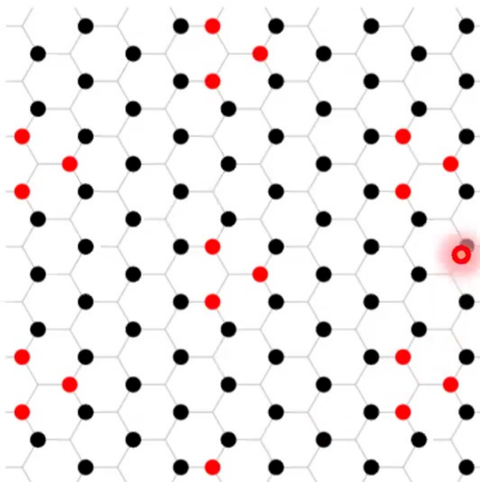
Attraction from pure electrostatic repulsion!

Lowest Energy-Per-Charge Excitation

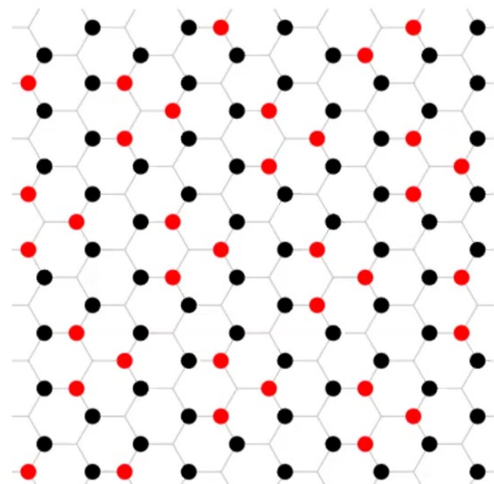


- E_d: energy of a charge-transfer dipole
- Phase diagram includes **all** V_{ij}

Pair Density Waves



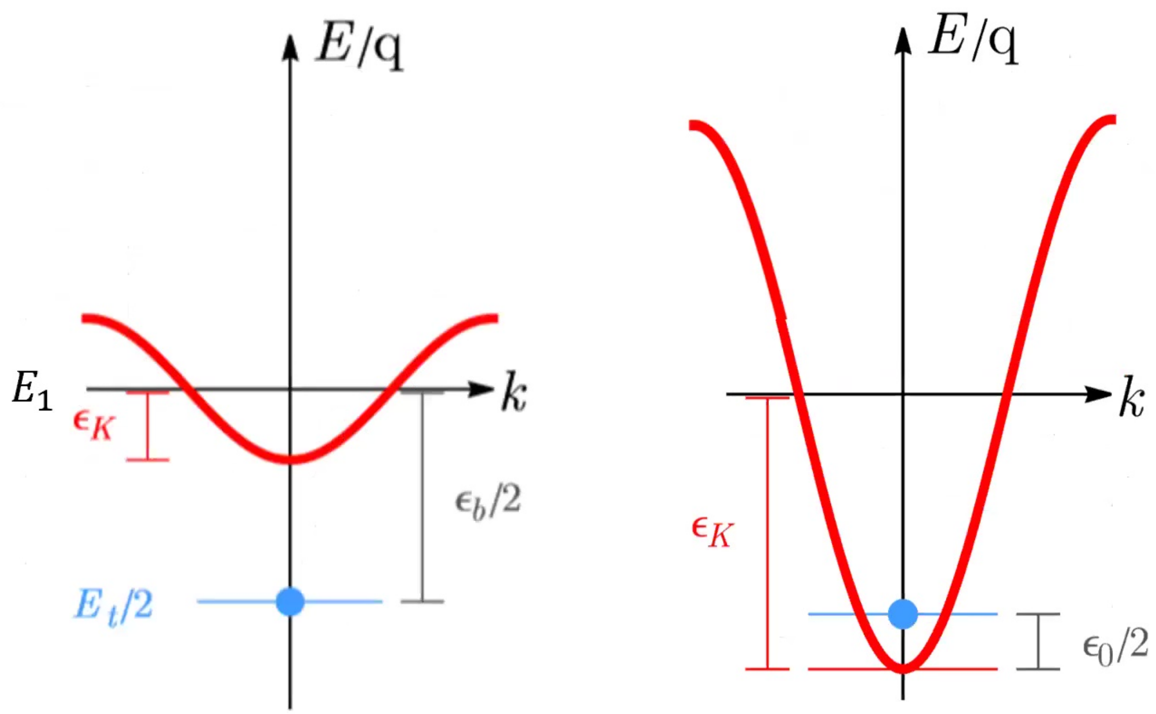
(b) $\delta = 1/8 = 0.125$
$q = 2, r_1 = 4, r_2 = 0$



(d) $\delta = 2/7 \approx 0.286$
$q = 2, r_1 = 2, r_2 = 1$

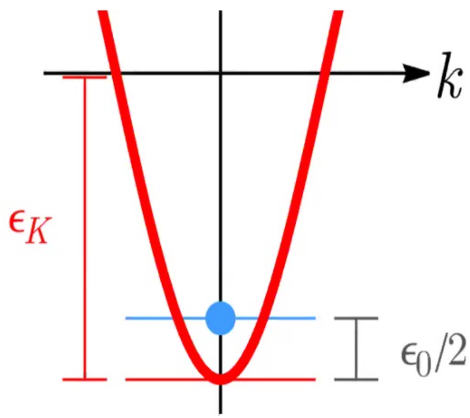
Densest packing of trimers without costing additional interactions $V_{n\leq 4}$

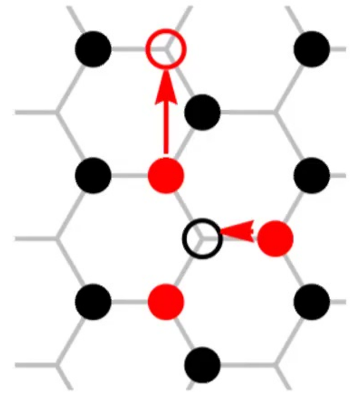
Increasing Electron Hopping



As the bandwidth increases, the energy of a delocalized hole at the bottom of band is lowered towards $E_t/2$.

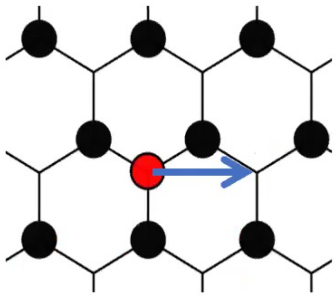
Hole-Trimer Resonance





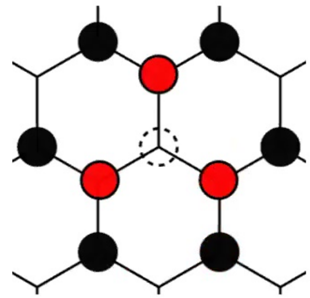
When the energy of a delocalized hole approaches $E_t/2$, trimer and hole interact resonantly (Feshbach resonance in *many-body* "vacuum").

Hole-Trimer Conversion



$t > 0$

- Band of doped holes have degenerate minima at $\pm K$ (valley pseudospin)



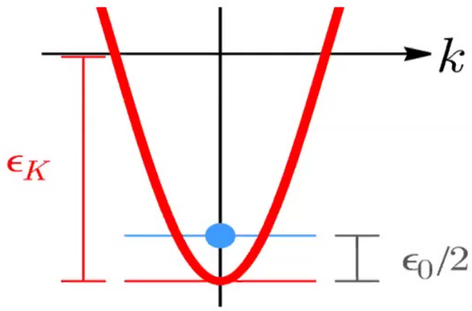
- Spin-polarized trimer state is odd under reflection

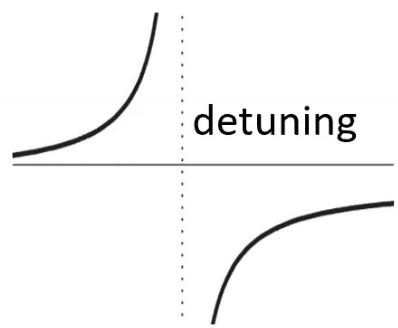
Trimer can convert into two delocalized holes of the same spin in s-wave pseudospin-singlet state

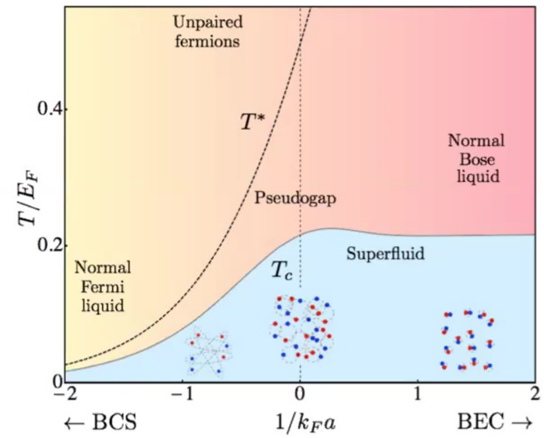
$$g\left(\phi\psi_+^\dagger\psi_-^\dagger + \phi^\dagger\psi_-\psi_+\right)$$

Resonantly Paired Superconductor

Bose-Fermi model for doped charge-transfer insulator:







Gurarie & Radhovsky, Randeria & Taylor …

As the detuning approaches zero, scattering length diverges, regardless of the Coulomb repulsion. Then, immediately upon doping, the ground state is a superconducting state of hole-trimer mixture.

3-Particle Mechanism for Superconductivity

Valentin Crepal
(MIT)

arXiv:2012.08528

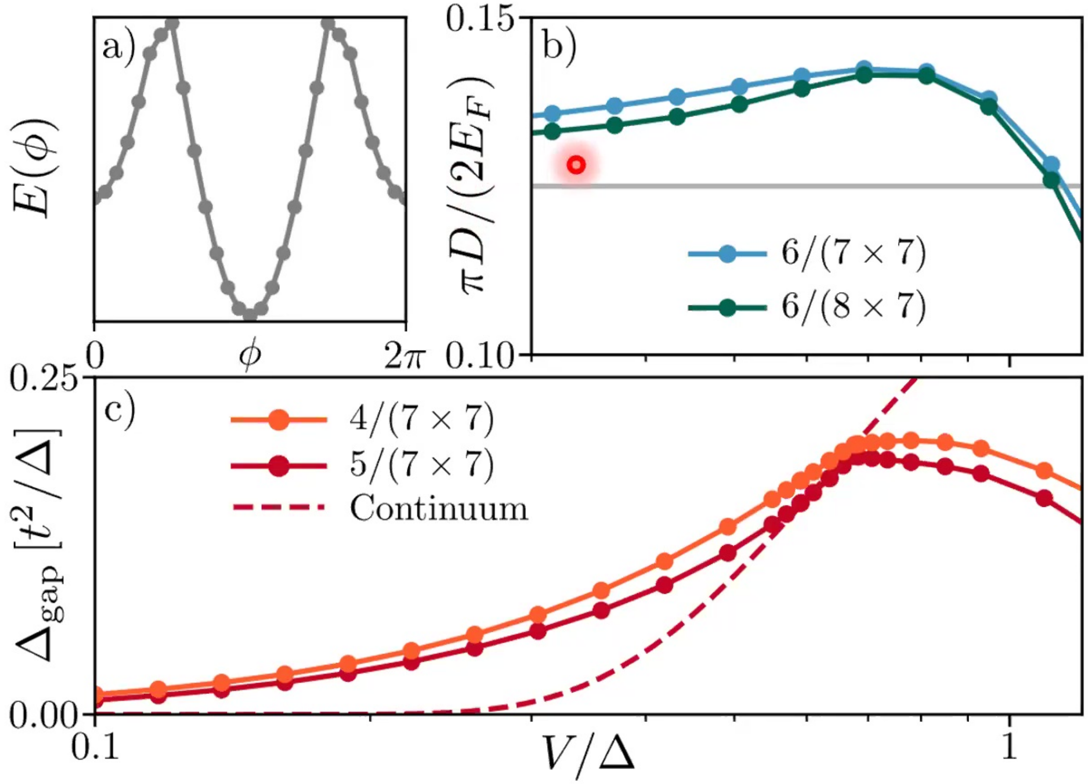
arXiv:2103.12060

Kevin Slagle
(Caltech)

PRB 102, 235423 (2020)

Everything you want to know about this theory

Exact Diagonalization



Charge stiffness : $D = \frac{1}{16\pi^2}\,\frac{L_1}{L_2}\,\frac{\partial^2 E(N,\phi)}{\partial\phi^2}\Big|_{\phi=0}$

Pairing gap : $\Delta_{\mathrm{gap}} = \frac{(-1)^N}{2}\left[E(N+1)+E(N-1)-2E(N)\right]$