Quantum Metric and Correlated States in Two Dimensional Systems

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WILLIAM & MARY
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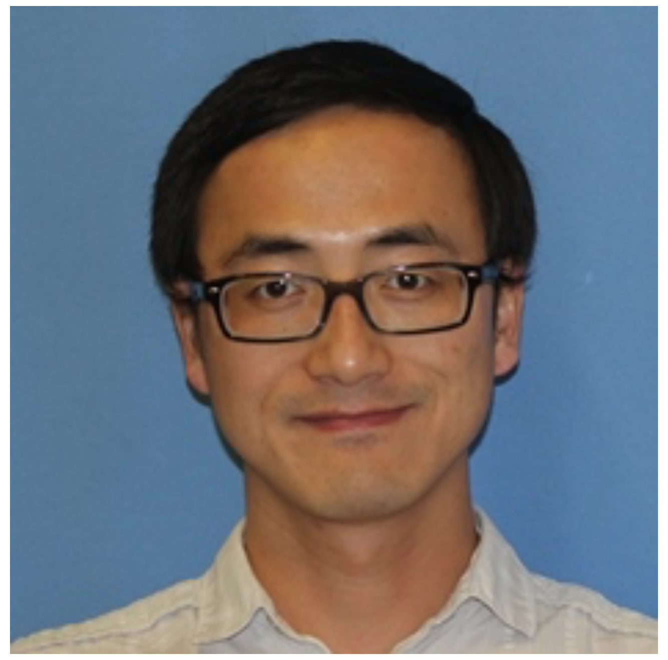

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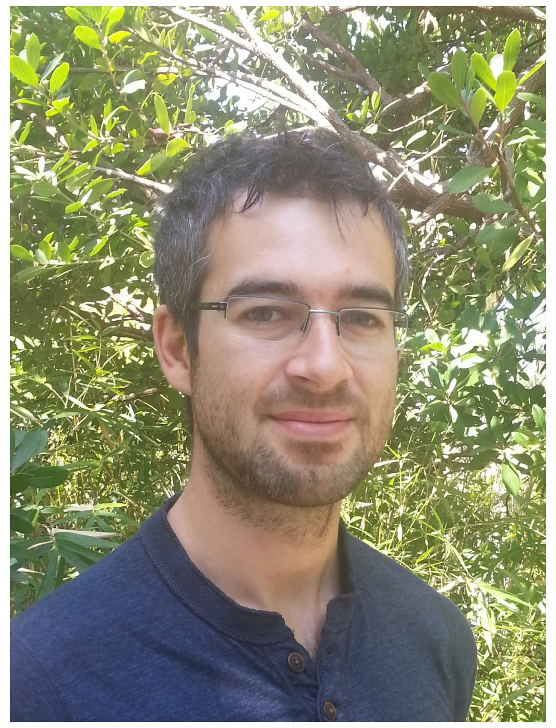

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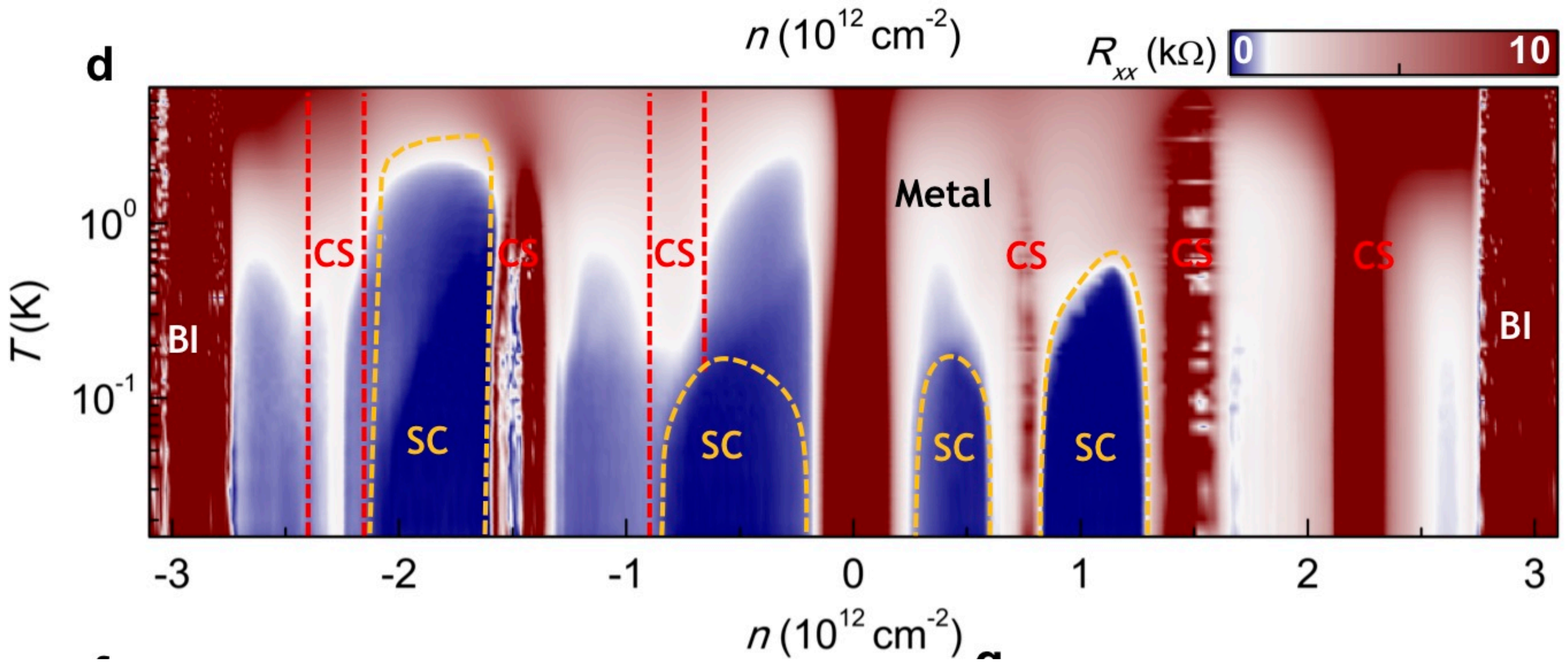
Motivation

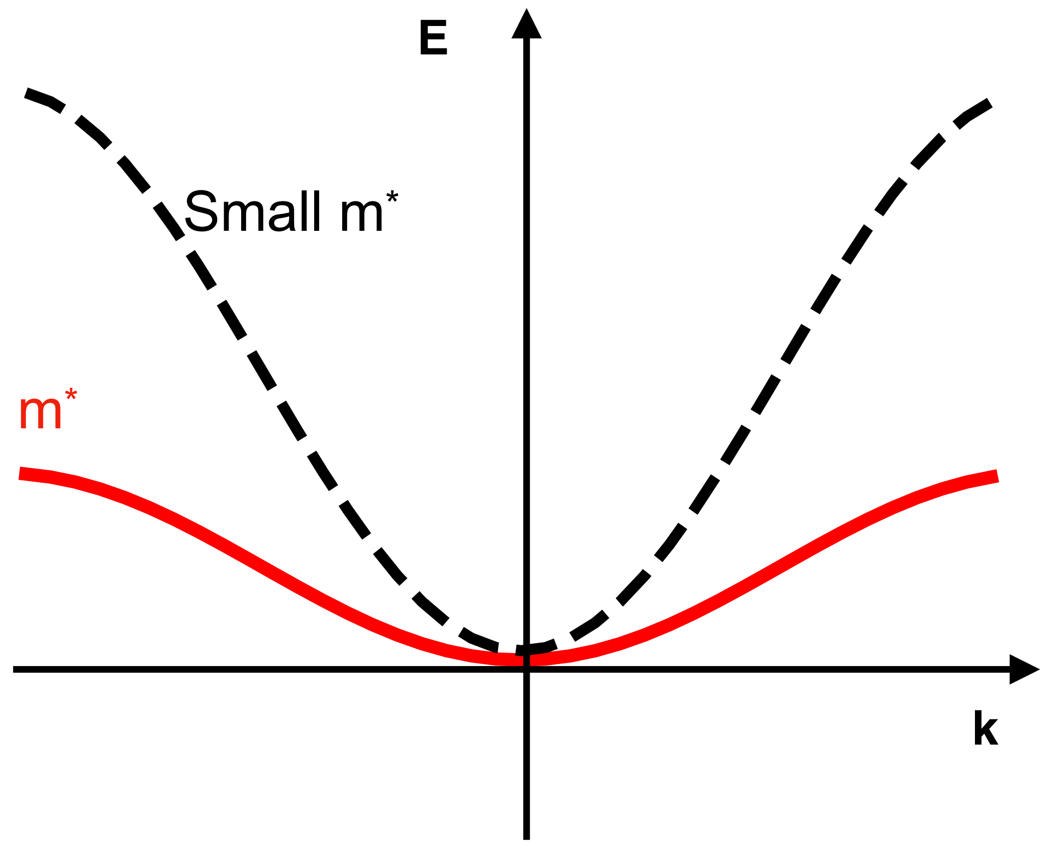
Xiaobo Lu et al. Nature (2019)



$$T_c \propto \exp\left(-\frac{1}{|U|\rho_0(E_F)}\right)$$

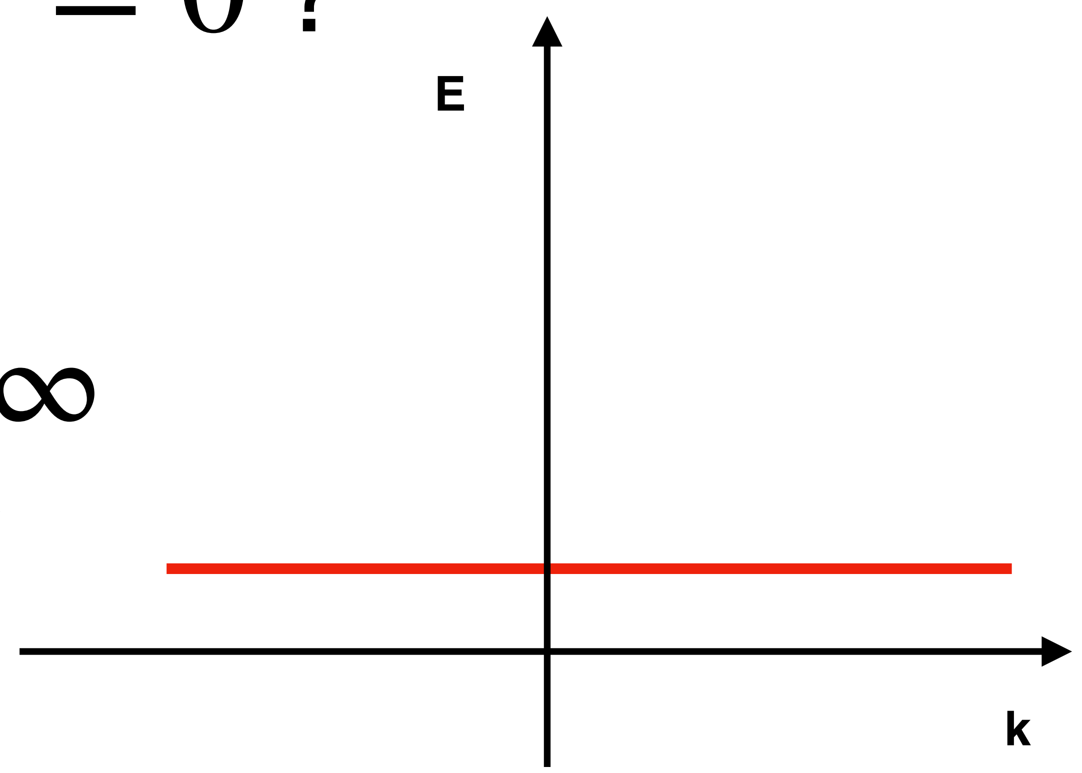
Conventional analysis tells us that the superconducting weight $D^{(s)}$ should scale as:

$$D^{(s)} = \frac{n}{m^*}$$



In the limit of m* —> ∞

$D^{(s)} = 0$?



Distance Between Vectors in Hilbert Space

Given a Hilbert space, $\mathscr{H}$, using the inner product we can define a distance between two vectors in $\mathscr{H}$. We can use **k** to parametrize the vectors.

$$|\Psi(\mathbf{k})\rangle; \quad |\Psi(\mathbf{k}+d\mathbf{k})\rangle \qquad\qquad ds^2 = (\langle\Psi(\mathbf{k}+d\mathbf{k})| - \langle\Psi(\mathbf{k})|)(|\Psi(\mathbf{k}+d\mathbf{k})\rangle - |\Psi(\mathbf{k})\rangle)$$

We can write

$$|\Psi(\mathbf{k}+dk_\mu)\rangle \approx |\Psi(\mathbf{k})\rangle + \underbrace{\partial_{k_\mu}|\Psi(\mathbf{k})\rangle}_{\partial_\mu|\Psi\rangle} dk^\mu$$

Using the fact that the vectors are normalized, $\langle\Psi|\Psi\rangle = 1$, we then find:

$$ds^2 = \underbrace{\langle\partial_\mu\Psi|\partial_\nu\Psi\rangle}_{M_{\mu\nu}} dk^\mu dk^\nu;$$

Symmetric part: $\gamma^{(s)}_{\mu\nu} \equiv \frac{1}{2}(M_{\mu\nu} + M_{\nu\mu});$

Antisymmetric part: $\gamma^{(a)}_{\mu\nu} \equiv \frac{1}{2}(M_{\mu\nu} - M_{\nu\mu});$

$$\langle\partial_\mu\Psi|\partial_\nu\Psi\rangle = \langle\partial_\nu\Psi|\partial_\mu\Psi\rangle^* \longrightarrow$$

$\gamma^{(s)}_{\mu\nu}$ is purely real

$\gamma^{(a)}_{\mu\nu}$ is purely imaginary. Let $\gamma^{(a)}_{\mu\nu} = iB_{\mu\nu}$

Quantum Geometric Tensor

Recall:

Berry connection: $\beta_\mu \equiv i\langle\Psi|\partial_\mu\Psi\rangle$

Berry curvature: $\Omega_{\mu\nu} \equiv \partial_\mu\beta_\nu - \partial_\nu\beta_\mu = 2\gamma^{(a)}_{\mu\nu} = 2iB_{\mu\nu}$

Consider gauge transformation

$$|\Psi(\mathbf{k})\rangle \to e^{i\alpha(\mathbf{k})}|\Psi(\mathbf{k})\rangle \longrightarrow$$

$B_{\mu\nu}$ is invariant;

$\gamma^{(s)}_{\mu\nu}$ is not: $\quad \gamma^{(s)}_{\mu\nu} \to \gamma^{(s)}_{\mu\nu} + (\beta_\mu - i\partial_\mu\alpha)(\beta_\nu - i\partial_\nu\alpha) - \beta_\mu\beta_\nu$

However, we can easily redefine $M_{\mu\nu}$ in a way that is gauge invariant and so useful to define the distance between two physical quantum states (rays in the projective Hilbert space $P_{\mathscr{H}}$):

$$M_{\mu\nu} \to Q_{\mu\nu} \equiv \langle\partial_\mu\Psi|\partial_\nu\Psi\rangle - \langle\partial_\mu\Psi|\Psi\rangle\langle\Psi|\partial_\nu\Psi\rangle;$$

$$Q_{\mu\nu} = g_{\mu\nu} + iB_{\mu\nu}$$

- $Q_{\mu\nu}$ ↑ Quantum Geometric Tensor
- $g_{\mu\nu}$ ↑ Real Part
- $B_{\mu\nu}$ ↑ Imaginary part Berry curvature

and so, considering that $B_{\mu\nu}$ is antisymmetric:

$$ds^2 = Q_{\mu\nu}dk^\mu dk^\nu = g_{\mu\nu}dk^\mu dk^\nu \longrightarrow$$ $g_{\mu\nu}$ Fubini-Study Quantum Metric

- $g_{\mu\nu}$ is the unique Riemannian metric on $P_{\mathscr{H}}$ that is invariant under unitary transformations

J.P. Provost, G. Vallee, Comm. Math. Phys. (1980)

- $Q_{\mu\nu}$ is positive semidefinite $\longrightarrow$
  - $\det g_{\mu\nu} \geq |B_{\mu\nu}|^2$
  - $\mathrm{Tr}g_{\mu\nu} \geq 2|B_{\mu\nu}|$

Rahul Roy PRB (2014)

Linear Current Response

Let's consider a system described by the Hamiltonian *H*, and study the current response due to an external vector field *A* (e=1):

$$j_\mu(\mathbf{k},\omega) = K_{\mu\nu}(\mathbf{k},\omega)A_\nu(\mathbf{k},\omega)$$

$K_{\mu\nu}$ has two contributions:

$$K_{\mu\nu}(\mathbf{k},\omega) = \langle T_{\mu\nu}\rangle + \langle \chi^p_{\mu\nu}(\mathbf{k},\omega)\rangle$$

Diamagnetic part

$$T_{\mu\nu} = \sum_\sigma \int \frac{d\mathbf{k}}{(2\pi)^d} c^\dagger_{\mathbf{k}\sigma}\partial_\mu\partial_\nu H(\mathbf{k},\sigma)c_{\mathbf{k}\sigma}$$

Paramagnetic part

$$\chi^p_{\mu\nu}(\mathbf{k},\omega) = -i\int_0^\infty dt e^{i\omega^+ t}\langle[j^p_\mu(\mathbf{k},t), j^p_\nu(-\mathbf{k},0)]\rangle$$

$$j^p_\mu(\mathbf{k}) = \sum_\sigma \int \frac{d\mathbf{k}`}{(2\pi)^d} c^\dagger_{\mathbf{k}'\sigma}\partial_\mu H(\mathbf{k}'+\mathbf{k}/2,\sigma)c_{\mathbf{k}'+\mathbf{k}\sigma}.$$

For a multi-orbital system, for the expectation values of the current operator $\partial_\mu \hat{H}$ we have:

$$\langle\Psi_n|(\partial_\mu\hat{H})|\Psi_m\rangle = \partial_\mu\epsilon_m\delta_{nm} + (\epsilon_m - \epsilon_n)\underbrace{\langle\Psi_n|\partial_\mu\Psi_m\rangle}$$

"Anomalous Contribution to the current"

Considering that K is a current-current correlator, this contribution, in turn, gives an additional purely quantum contribution to ρ_s

Drude Weight and Superfluid Weight

We want to consider the long-wavelength static limit. There are two ways to take this limit:

$$\lim_{\substack{\mathbf{k}=0 \\ \omega\to 0}} K_{\mu\nu}(\mathbf{k},\omega) = -\frac{D_{\mu\nu}}{\pi}; \longrightarrow \sigma_{\mu\nu} = D_{\mu\nu}\delta(\omega) + \sigma_{\mu\nu}^{(\text{regular})}(\omega)$$

↑ Drude weight

$$\lim_{\substack{\omega=0 \\ k_{\parallel}=0, \\ k_{\perp}\to 0}} K_{\mu\nu}(\mathbf{k},\omega) = -\frac{D^{(s)}_{\mu\nu}}{\pi}; \longrightarrow j_\mu = D^{(s)}_{\mu\nu} \lim_{k_\perp\to 0} A_\nu(k_\parallel = 0, \omega = 0)$$

Meissner Effect

↑ Superfluid Weight

$D \neq 0$, $D^{(s)} = 0$ } Metal

$D \neq 0$, $D^{(s)} \neq 0$ } Superconductor

$D = 0$, $D^{(s)} = 0$ } Insulator

For a single, isotropic, parabolic band, for $T \to 0$, we have

$$D = \frac{n}{m^*}; \qquad D^{(s)} = \frac{n}{m^*}.$$

D.J. Scalapino, S.R. White, S.C. Zhang
PRL (1992)

However, for a multiband system, we have a contribution to D and $D^{(s)}$ from the quantum metric.

Superfluid Weight in Multiband System

We start from BdG Hamiltonian (assume for TRS):

$$H_{\mathrm{BdG}} = \begin{pmatrix} H_T & \hat{\Delta} \\ \hat{\Delta}^\dagger & -H_B \end{pmatrix} \qquad H_{\mathrm{BdG}}|\psi_i\rangle = E_i|\psi_i\rangle$$

For $D^{(s)}$ we have:

$$D^{(s)}_{\mu\nu} = \sum_{i,j}\int \frac{d\mathbf{k}}{(2\pi)^d}\frac{n_F(E_i)-n_F(E_j)}{E_j-E_i}[\langle\psi_i|\partial_\mu H_{\mathrm{BdG}}|\psi_j\rangle\langle\psi_j|\partial_\nu H_{\mathrm{BdG}}|\psi_i\rangle - \langle\psi_i|\partial_\mu H_{\mathrm{BdG}}\tau_z|\psi_j\rangle\langle\psi_j|\tau_z\partial_\nu H_{\mathrm{BdG}}|\psi_i\rangle]$$

For the case of a well isolated band:

$$D^{(s)}_{\mu\nu} = \underbrace{\int\frac{d\mathbf{k}}{(2\pi)^d}\left[2\frac{\partial n_F(E_j)}{\partial E_j} + \frac{1-2n_F(E_j)}{E_j}\right]\frac{\Delta^2}{E_j^2}\partial_\mu\epsilon_j\partial_\nu\epsilon_j}_{\text{conventional contribution}} + \underbrace{2\Delta^2\int\frac{d\mathbf{k}}{(2\pi)^d}\frac{1-2n_F(E_j)}{E_j}g^{(j)}_{\mu\nu}}_{\text{geometric contribution}}$$

The flatter the bands the more relevant is the geometric contribution. For a 2D, flat, isolated band:

$$D^{(s)}_{\mu\nu} = 2\Delta\sqrt{\nu(1-\nu)}\int\frac{d\mathbf{k}}{(2\pi)^2}g_{\mu\nu}(\mathbf{k}).$$

$$\det g_{\mu\nu} \geq |B_{\mu\nu}|^2 \longrightarrow D^{(s)}_{\mu\nu} \geq \frac{\Delta}{\pi}\sqrt{\nu(1-\nu)}|C|$$

P.Törmä, S. Peotta, Nat. Comm. (2015). L. Liang et al. PRB (2017)

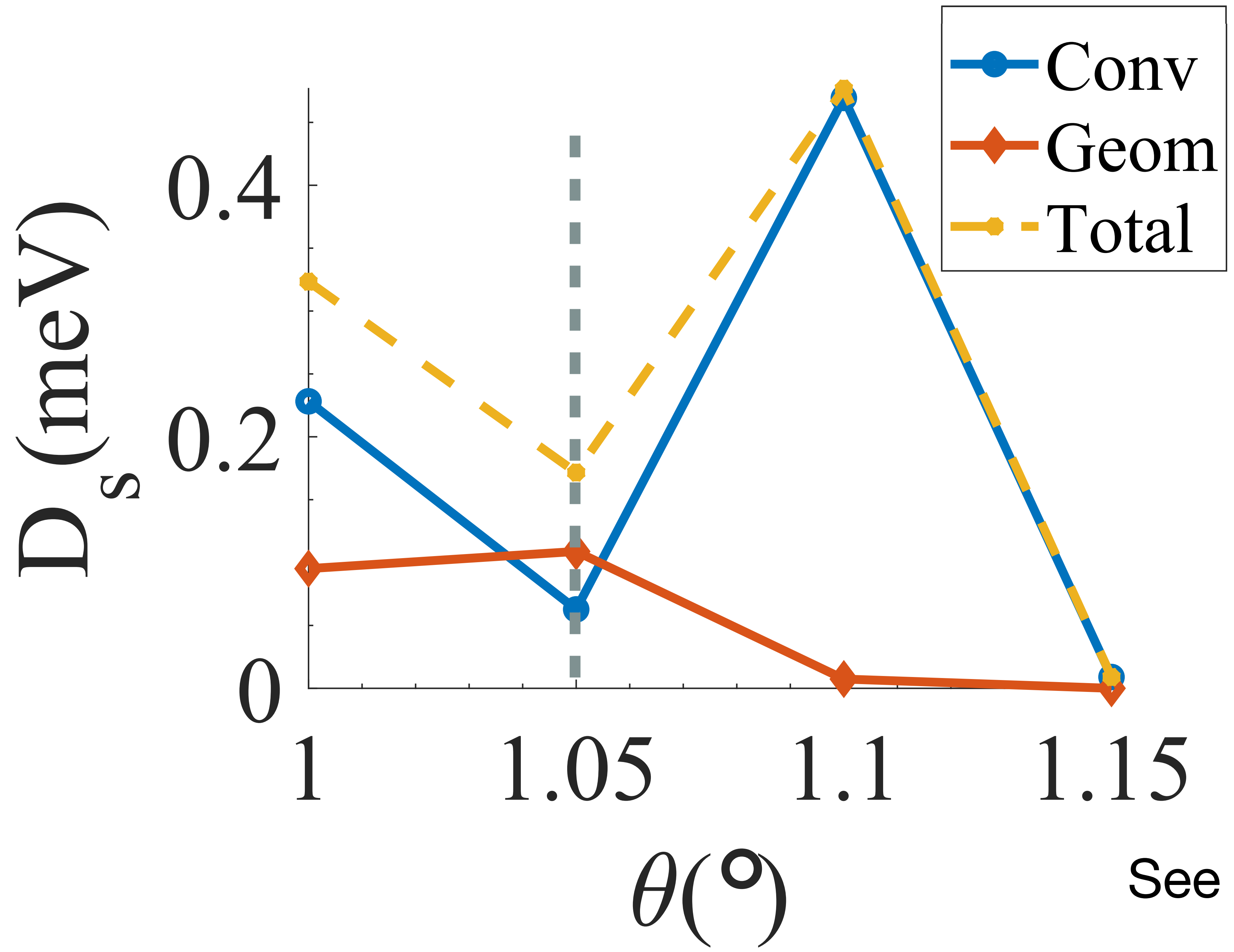
Superfluid Weight in TBLG

We assume simple s-wave pairing and fix Δ to agree with measured T_c

$$H_{\rm BdG} = \begin{bmatrix} H_{\rm TBLG,\mathbf{K}}(\mathbf{k}) & \hat{\Delta}_s \\ \hat{\Delta}_s^\dagger & -H^T_{\rm TBLG,\mathbf{K}'}(-\mathbf{k}) \end{bmatrix}, \qquad \hat{\Delta}_s = \Delta\tau_0 \sum_{\mathbf{b}} \Delta_{\mathbf{b}} e^{i\mathbf{b}\cdot\mathbf{r}},$$

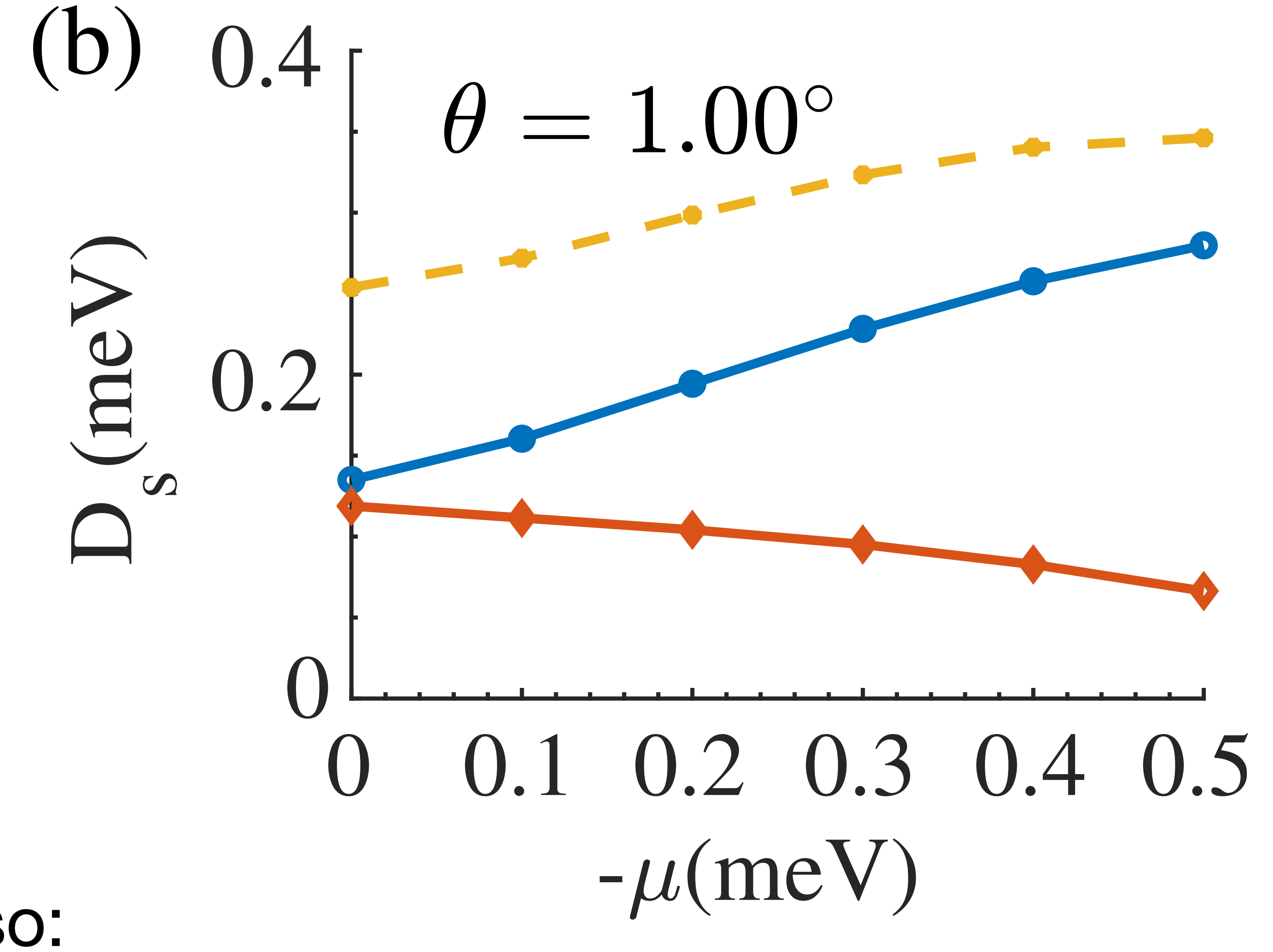
we find the coefficients $\Delta_{\mathbf{b}}$ solving the linearized gap equation. For our settings $\theta_{\rm magic} = 1.05^{\rm o}$

With some algebra we can separate the conventional and geometric contribution to $D^{(s)}$ (see Xu et al. PRL (2019)

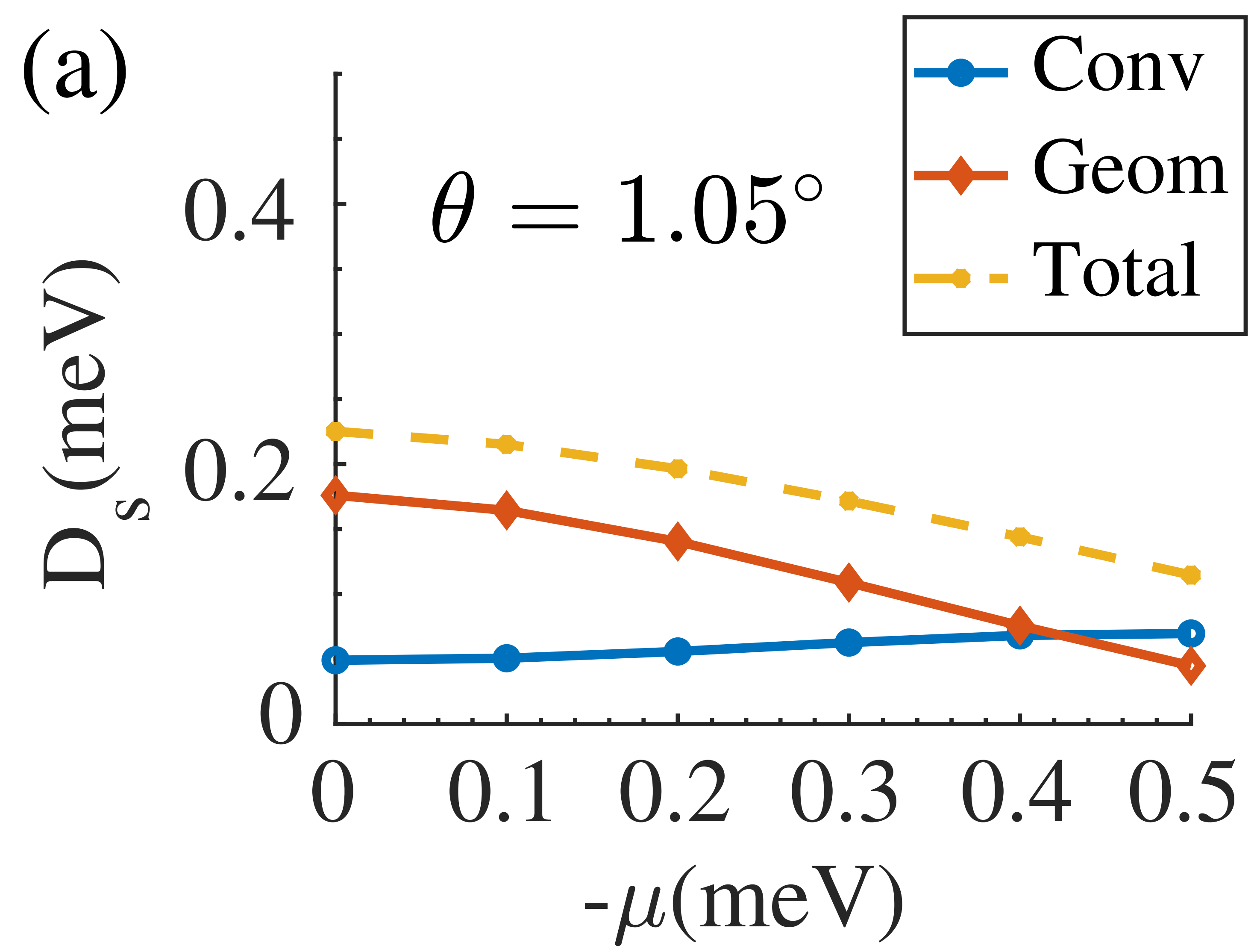


X.Hu, T. Hyart, D.Pikulin, ER. PRL (2019)

Away from magic angle, 1.00^0



At magic angle, 1.05^0



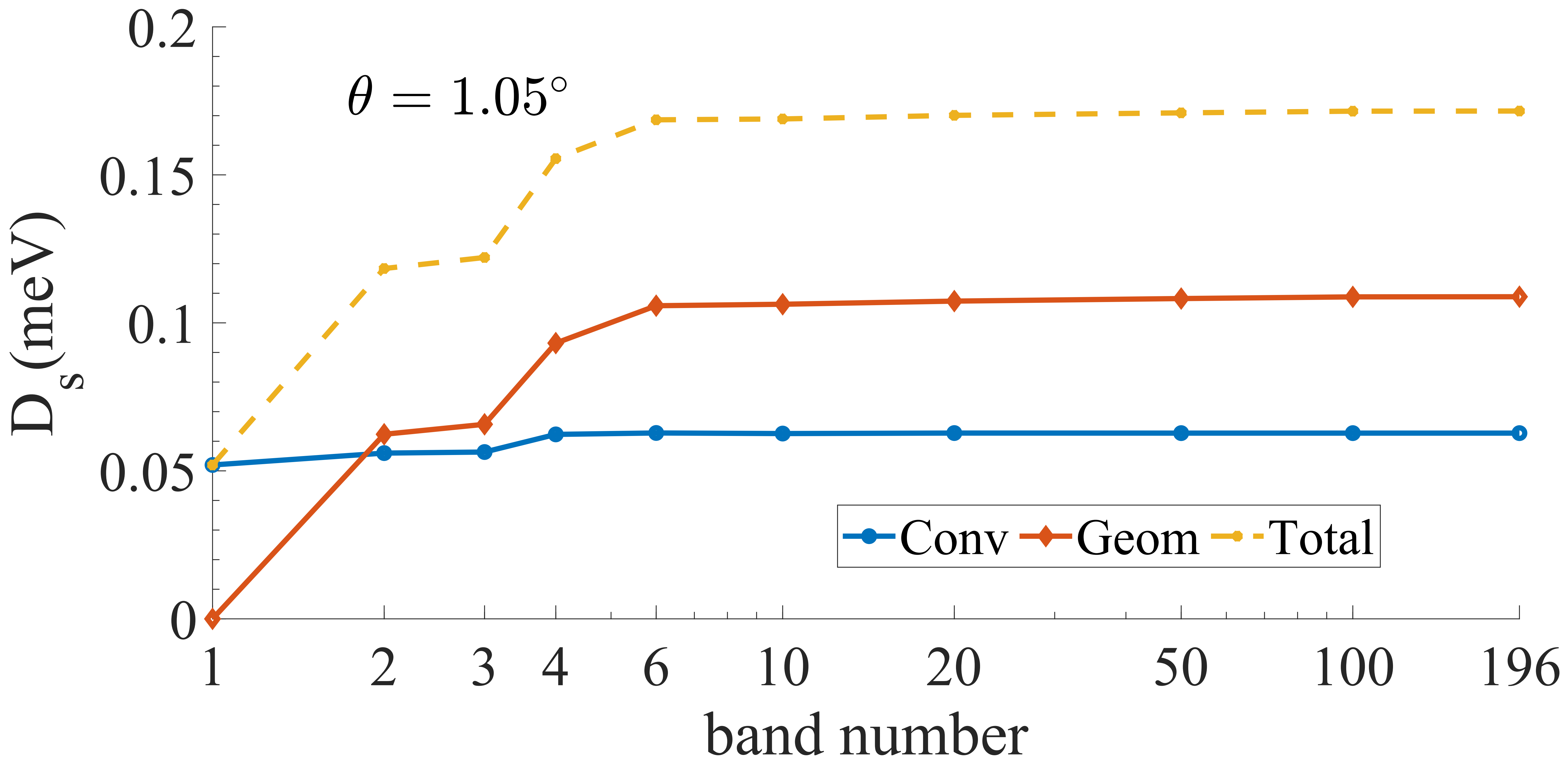
See also:

F. Xie et al. PRL (2020)
A. Julku et al PRB(2020)

P.Törmä, S. Peotta, B.A. Bernevig, Nat. Rev. Phys.(2022)
ER arXiv:2108.11478 (2021)

Dependence of $D^{(s)}$ on number of bands included

Superconducting TBLG



Berezinskii-Kosterlitz-Thouless Transition

In 2D, for a system whose ground state spontaneously breaks a U(1) symmetry, the thermodynamic transition from “ordered” to disordered phase is Berezinskii-Kosterlitz-Thouless transition. At T=T_{BKT} the thermal fluctuations are strong enough to unbind vortices -> the system stops being a superfluid.

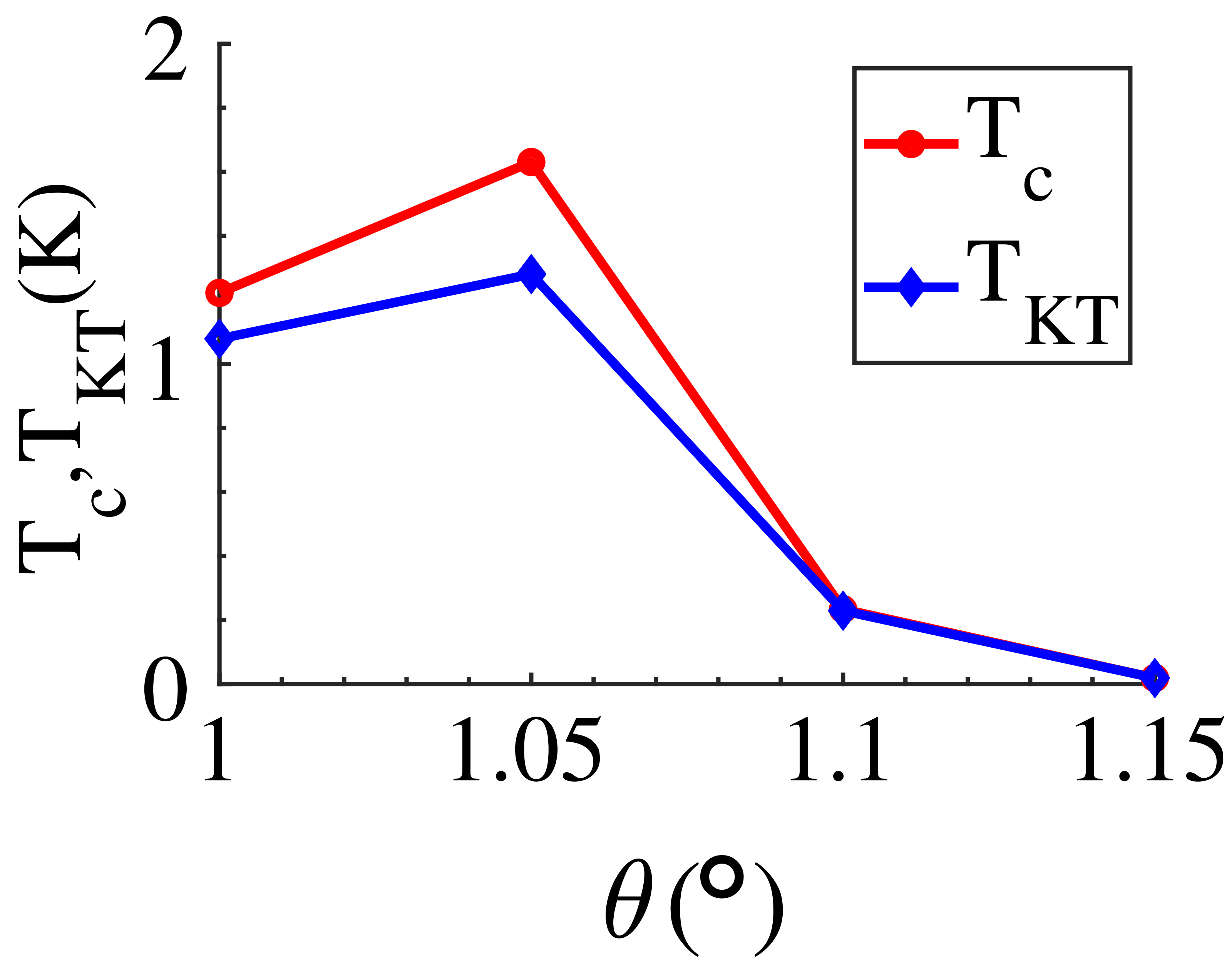
$$k_B T_{\mathrm{KT}} = \pi D^s[\Delta(T_{\mathrm{KT}}), T_{\mathrm{KT}}]$$

By calculating the temperature dependence of $D^{(s)}$ we can obtain T_{BKT}. In 2D $\rho^{(s)}$ is difficult to measure directly and so the measurement of T_{BKT} is a way to probe the quantum metric properties of the system. Notice that for the conventional case

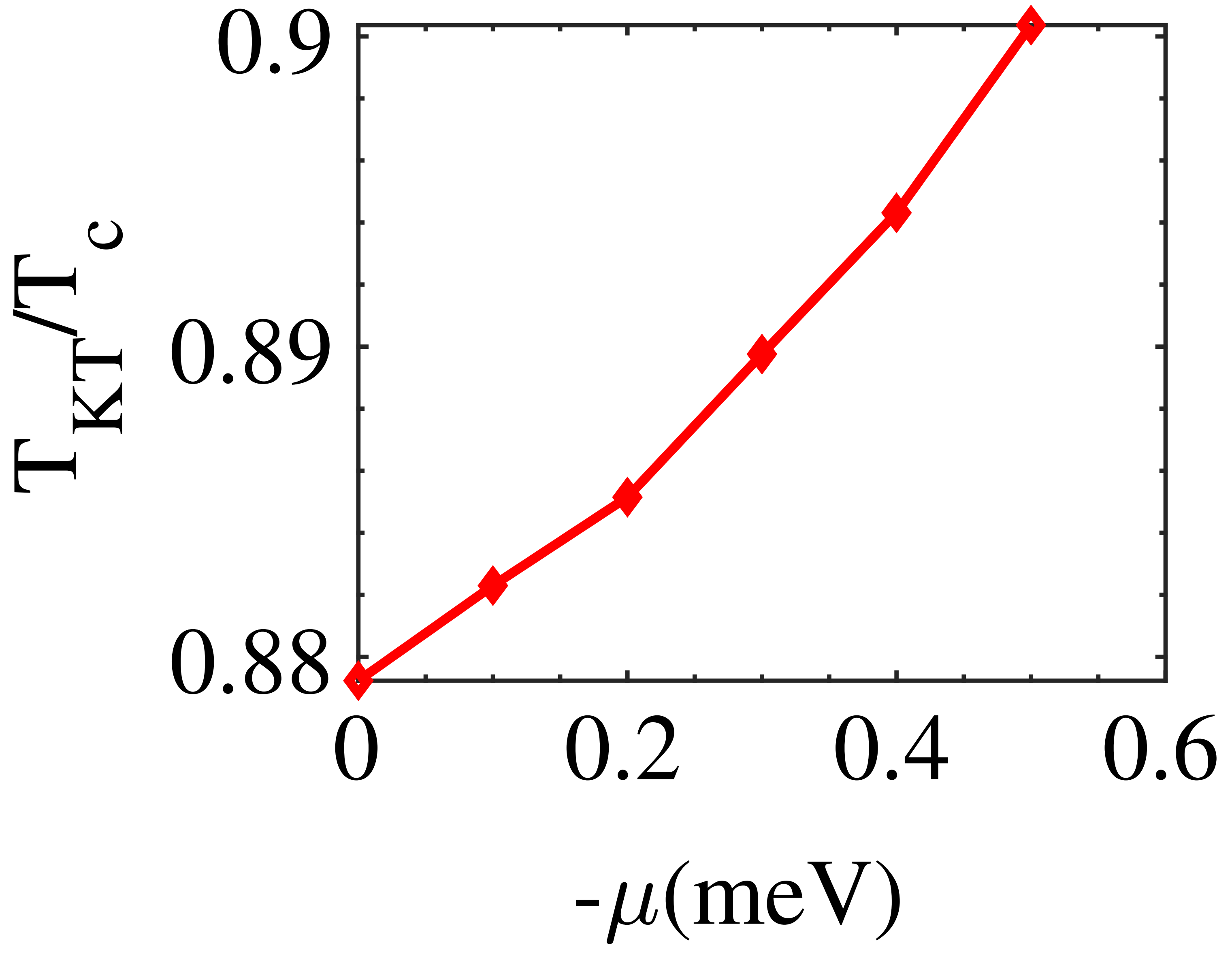
$D^{(s)}$ grows with density/chemical potential => T_{BKT} also grows with density/chemical potential

An opposite trend is a strong signature of the importance of the geometric contribution to $D^{(s)}$.

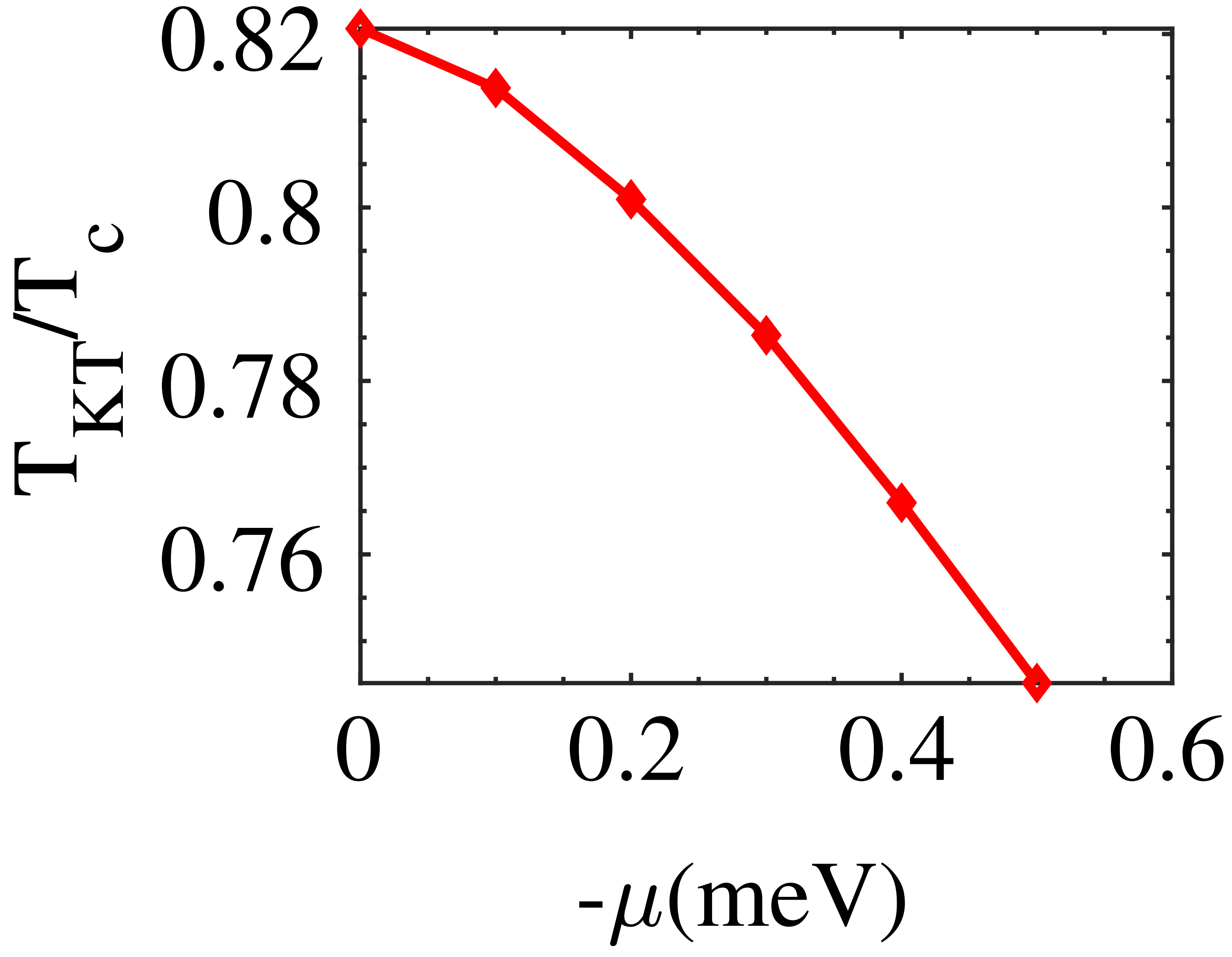
Berezinskii-Kosterlitz-Thouless Temperature



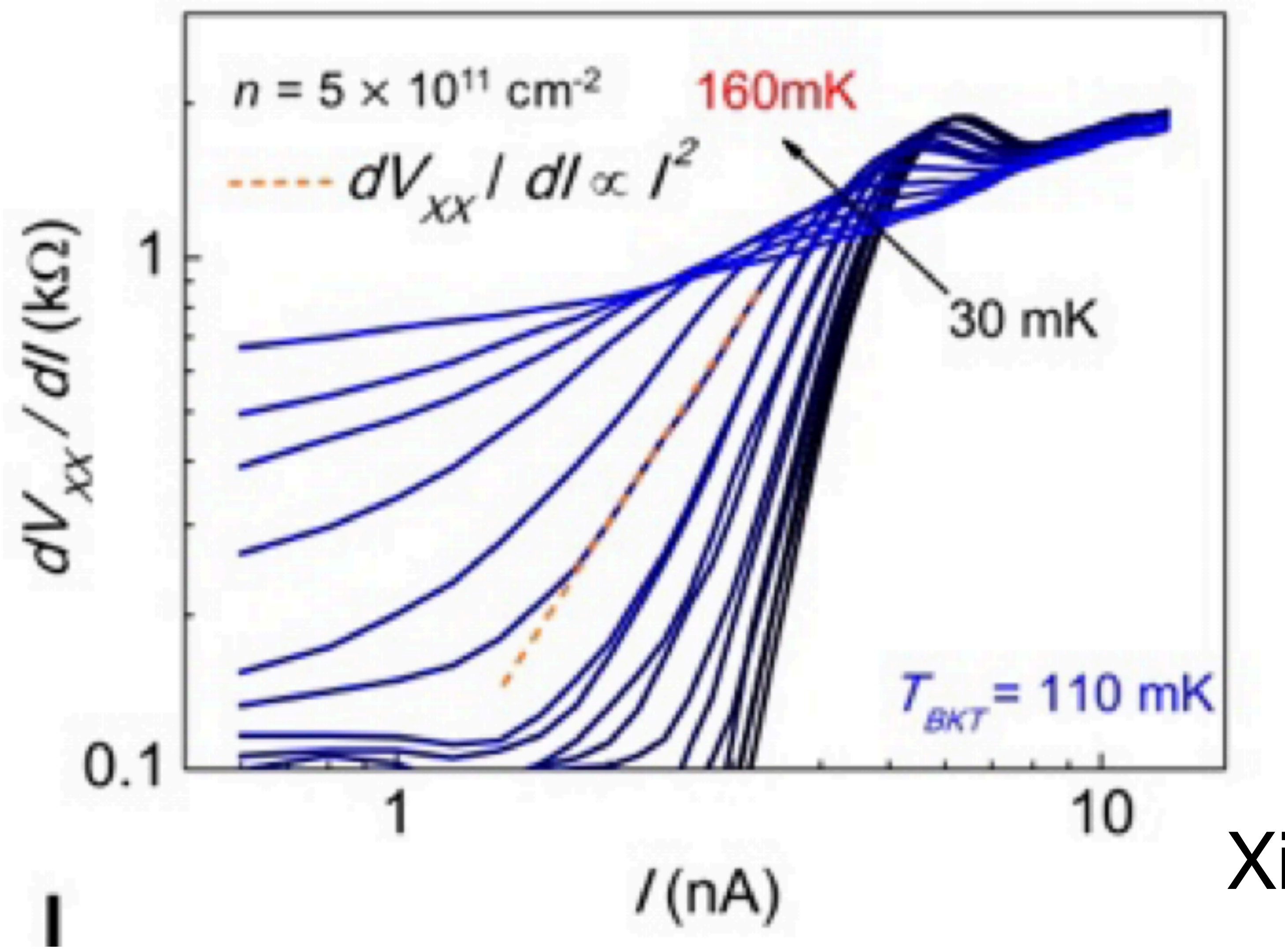
Away from magic angle, 1.00^0



At magic angle, 1.05^0

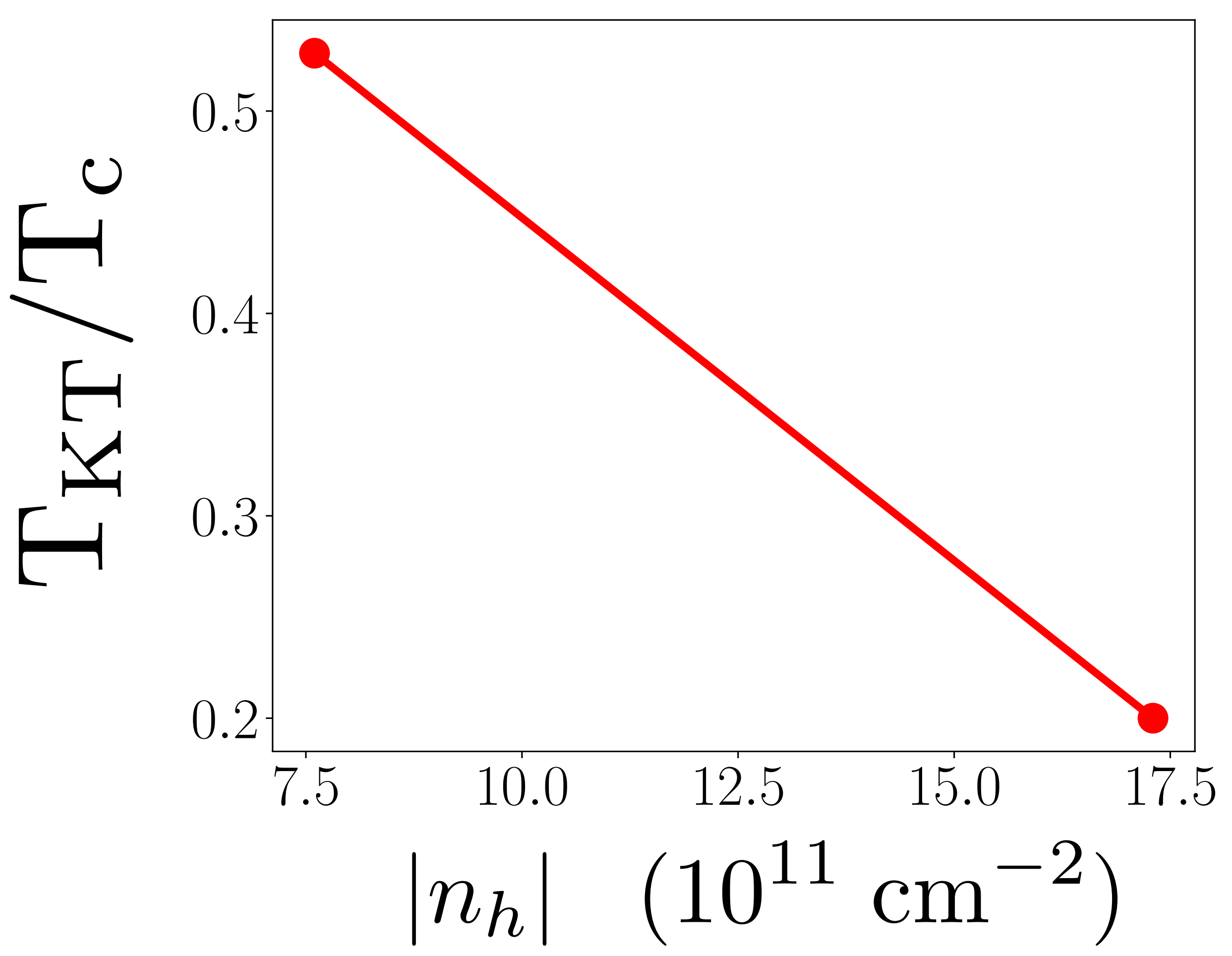


Xiang Hu et al. PRL (2019)



Xiao Lu et al. Nature (2019)

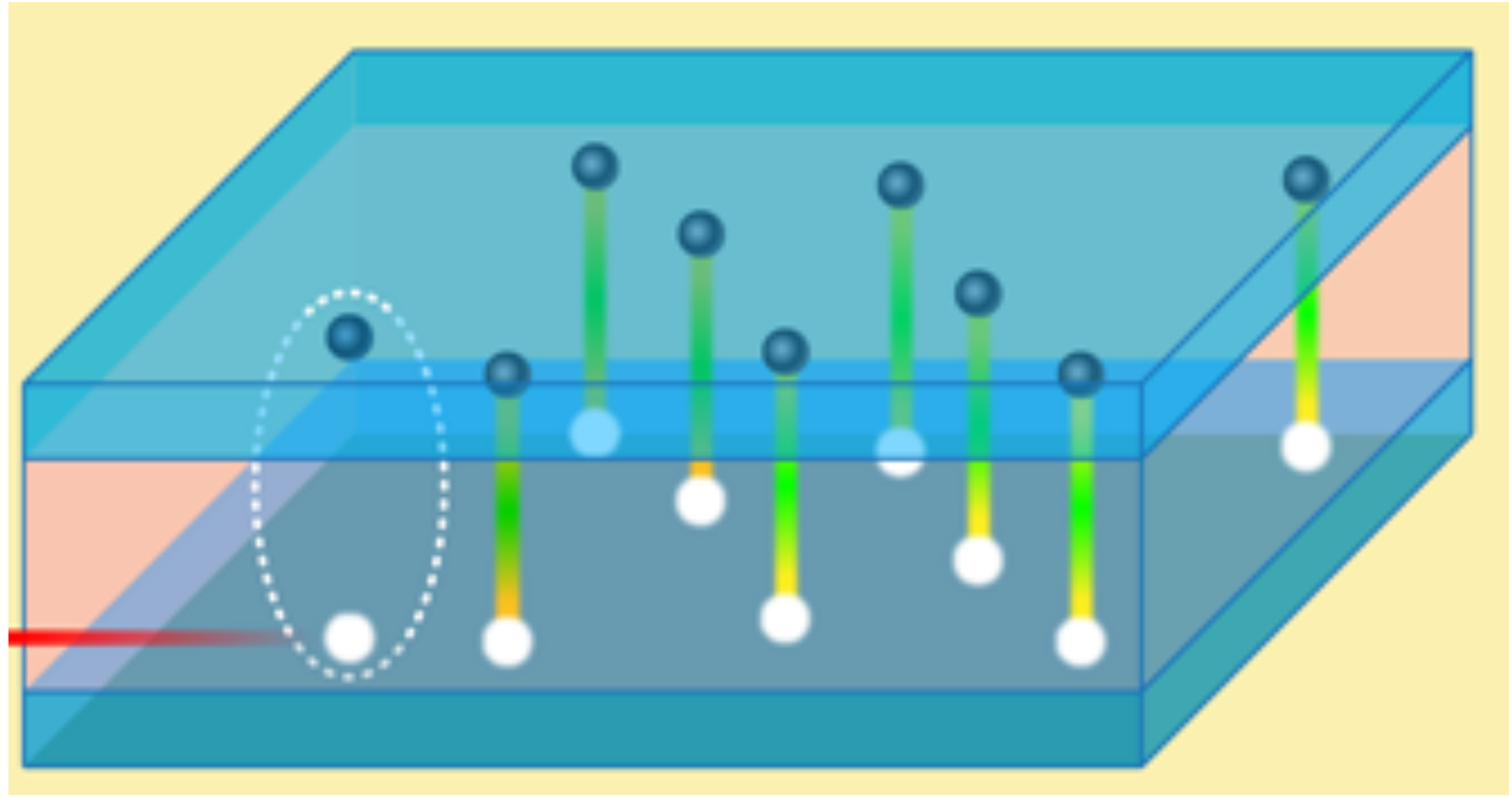
Extracting T_{BKT} for different dopings



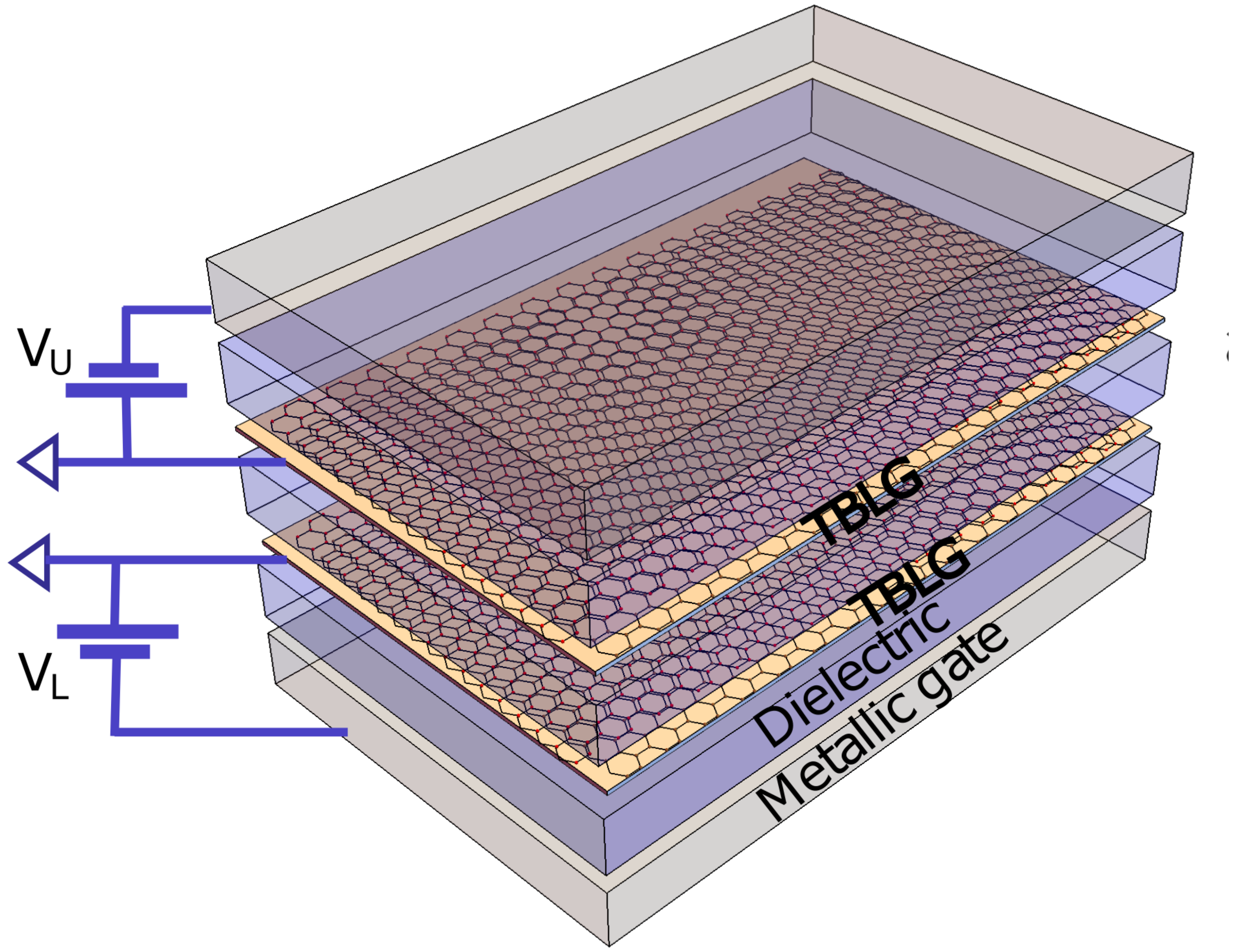
Exciton Condensate Superfluid

The connection between “stiffness” and quantum metric is general and can be applied to other ground states that break continuous symmetries, like ferromagnetic states, “orbital ferromagnetic” states whose signatures have been observed in TBLG.

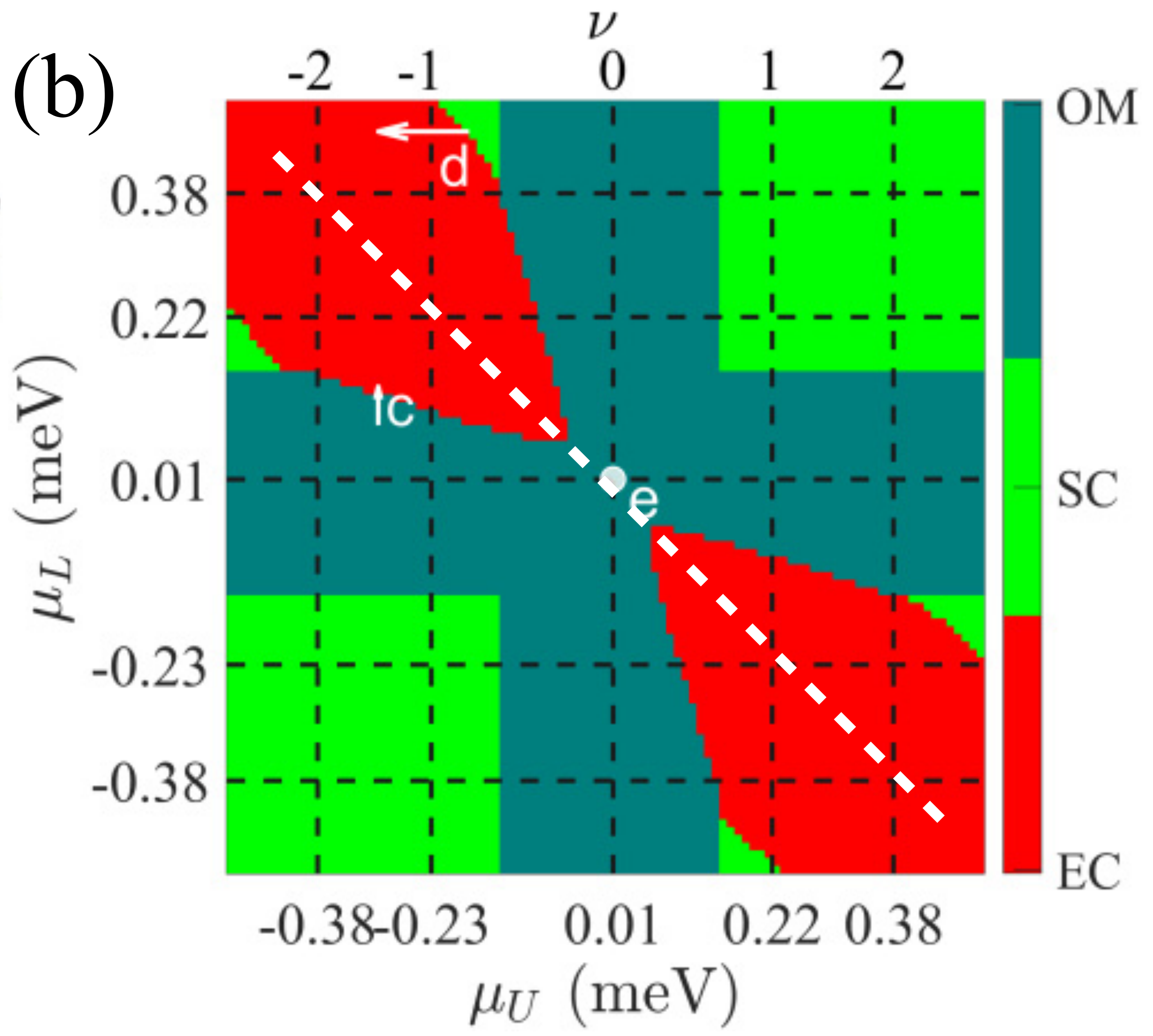
A particularly interesting state is the exciton condensate in bilayers.

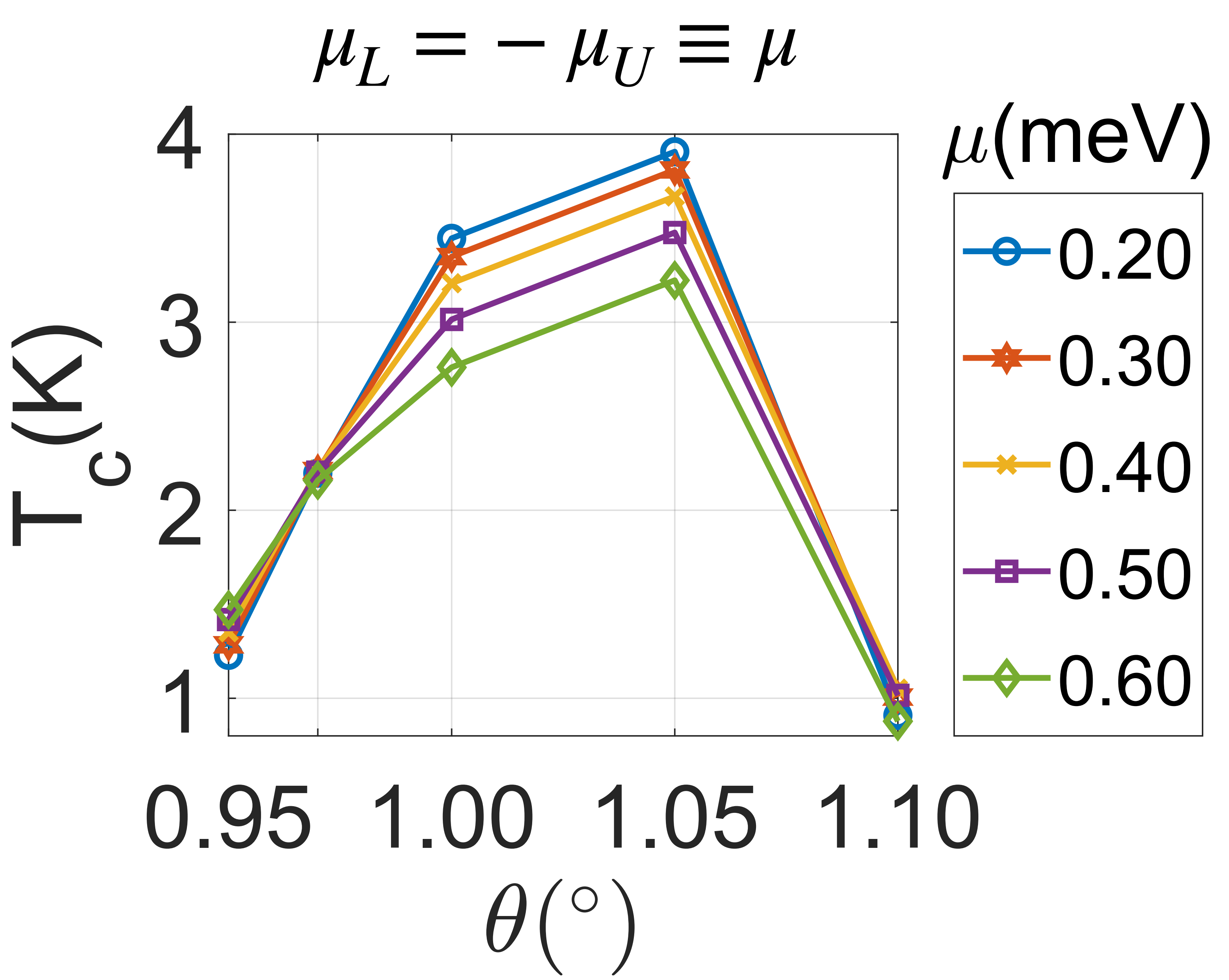


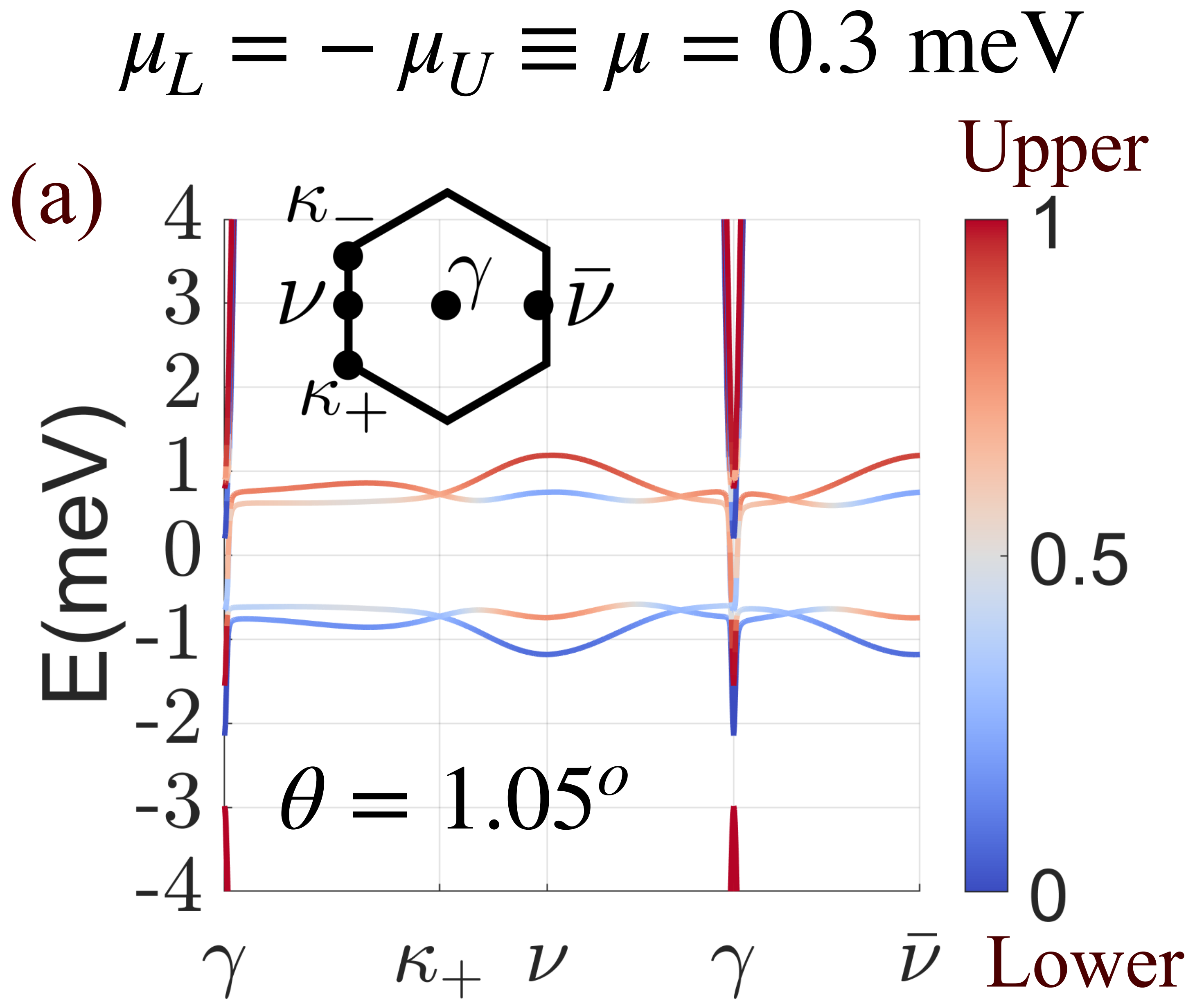
TBLG having almost flat bands seems a good candidate to realize an exciton condensate



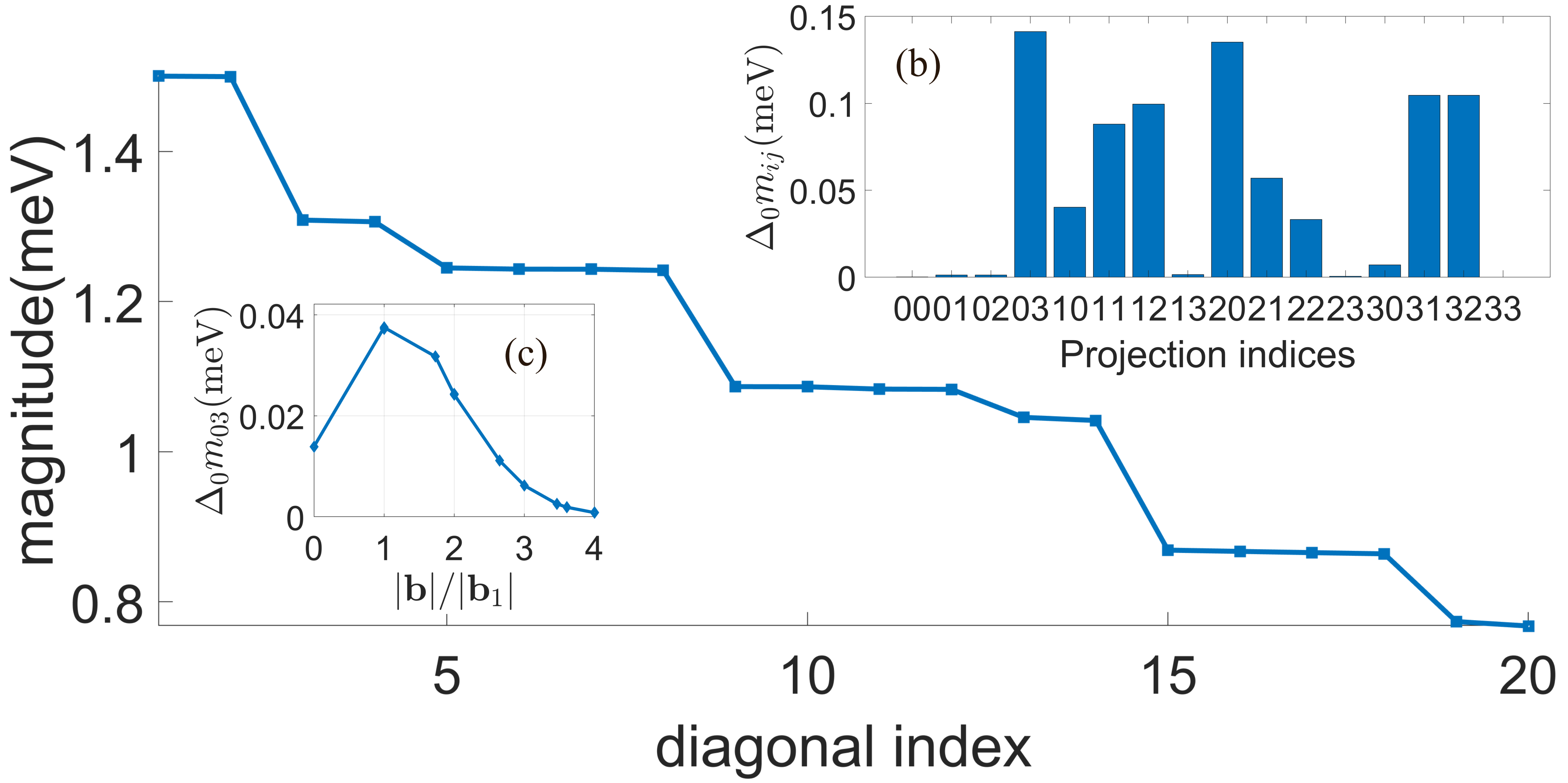
Double TBLG: phase diagram







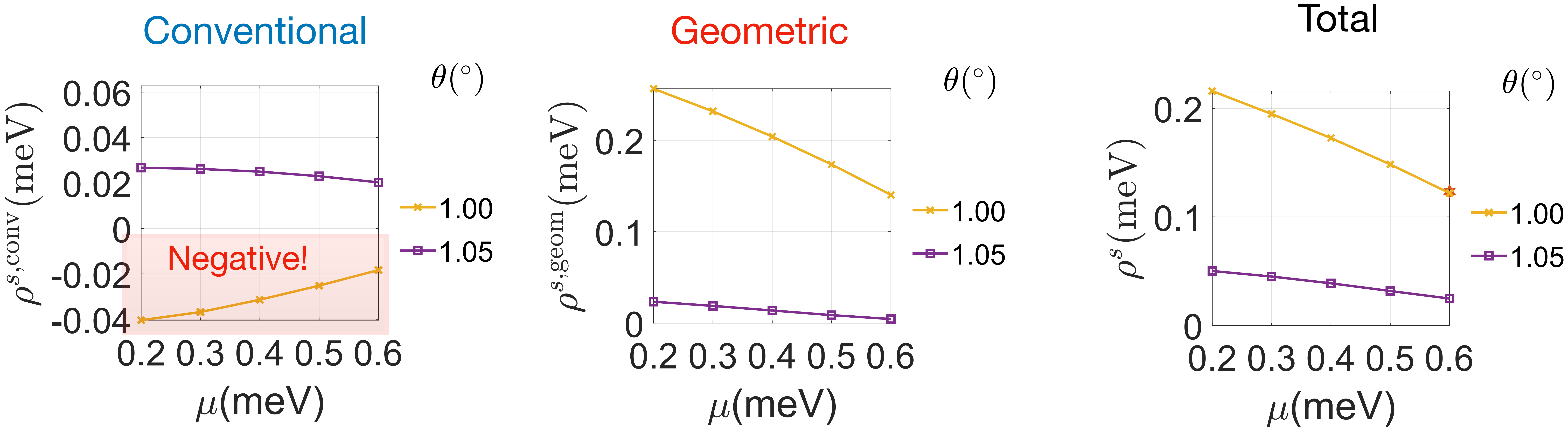
V_{0M}=130 meV, V_{SC}=75 meV, V_{EC}=60 mev

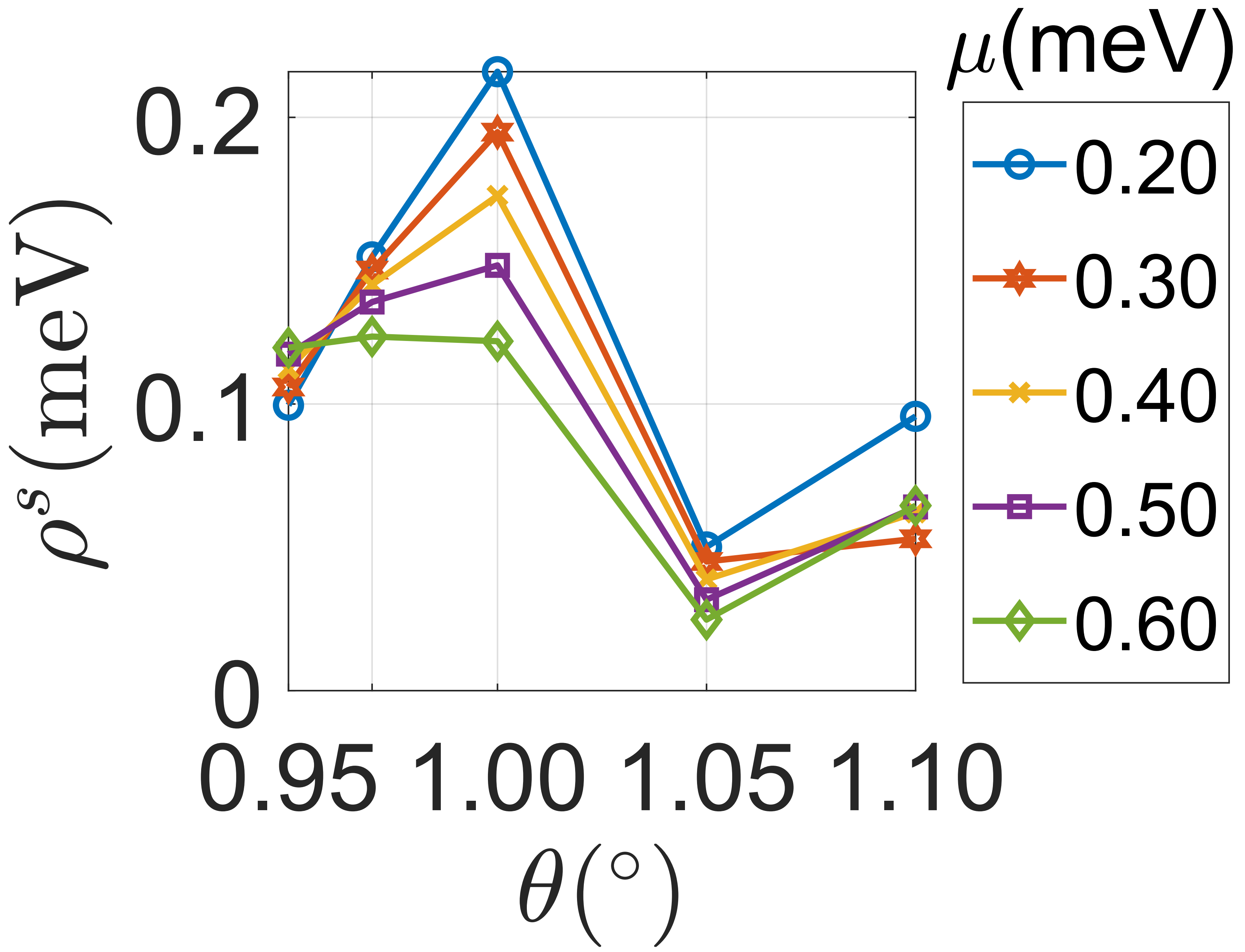


- For $\mu_L = -\mu_U$ exciton condensate is favored
- It's a truly multicomponent order parameter
- T_c is maximum at the magic angle as we would expect

X.Hu et al. PRB(L) (2022)

Double TBLG: Superfluid Stiffness

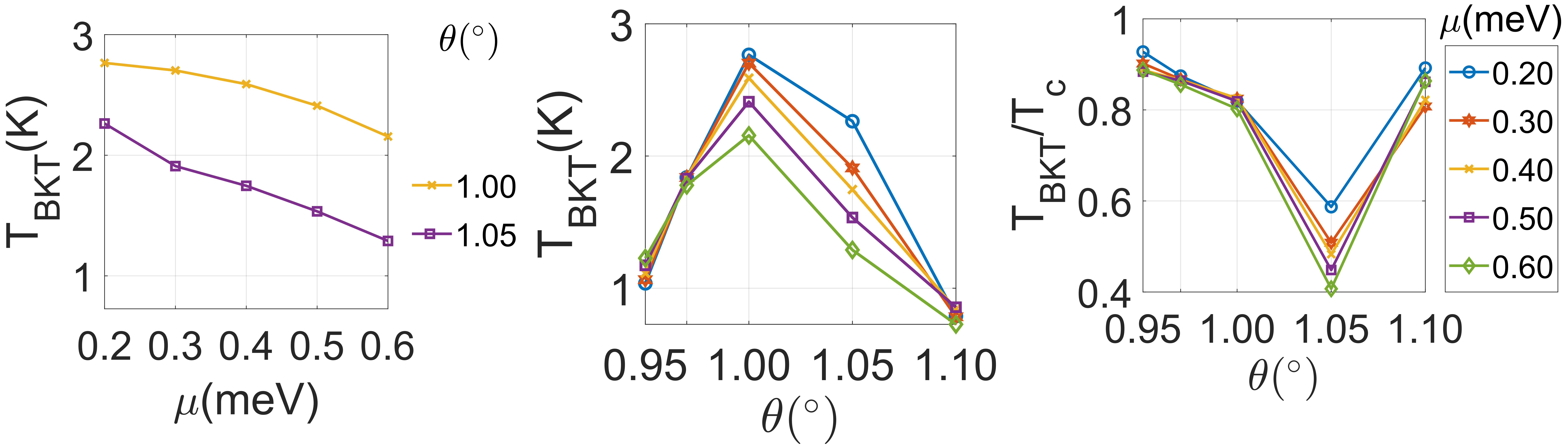




- Based on T_c TBLG is a great system to realize an exciton condensate
- Conventional treatment of ρ_s lead to conclusion that in TBLG the exciton condensate is not robust or very unstable
- The geometric contribution to ρ_s is essential for stability of condensate.

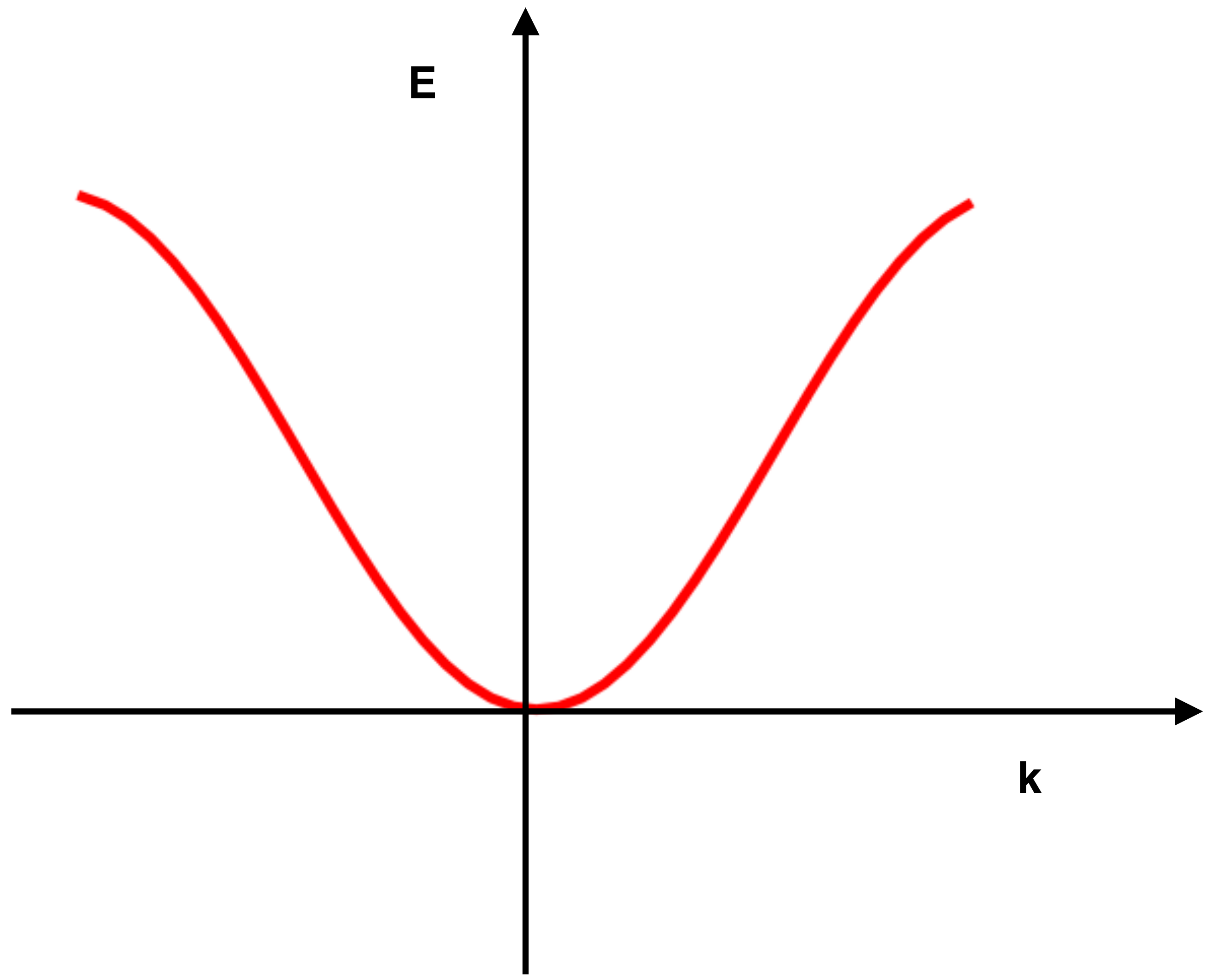
X.Hu et al. PRB(L) (2022)

Berezinskii-Kosterlitz-Thouless Temperature

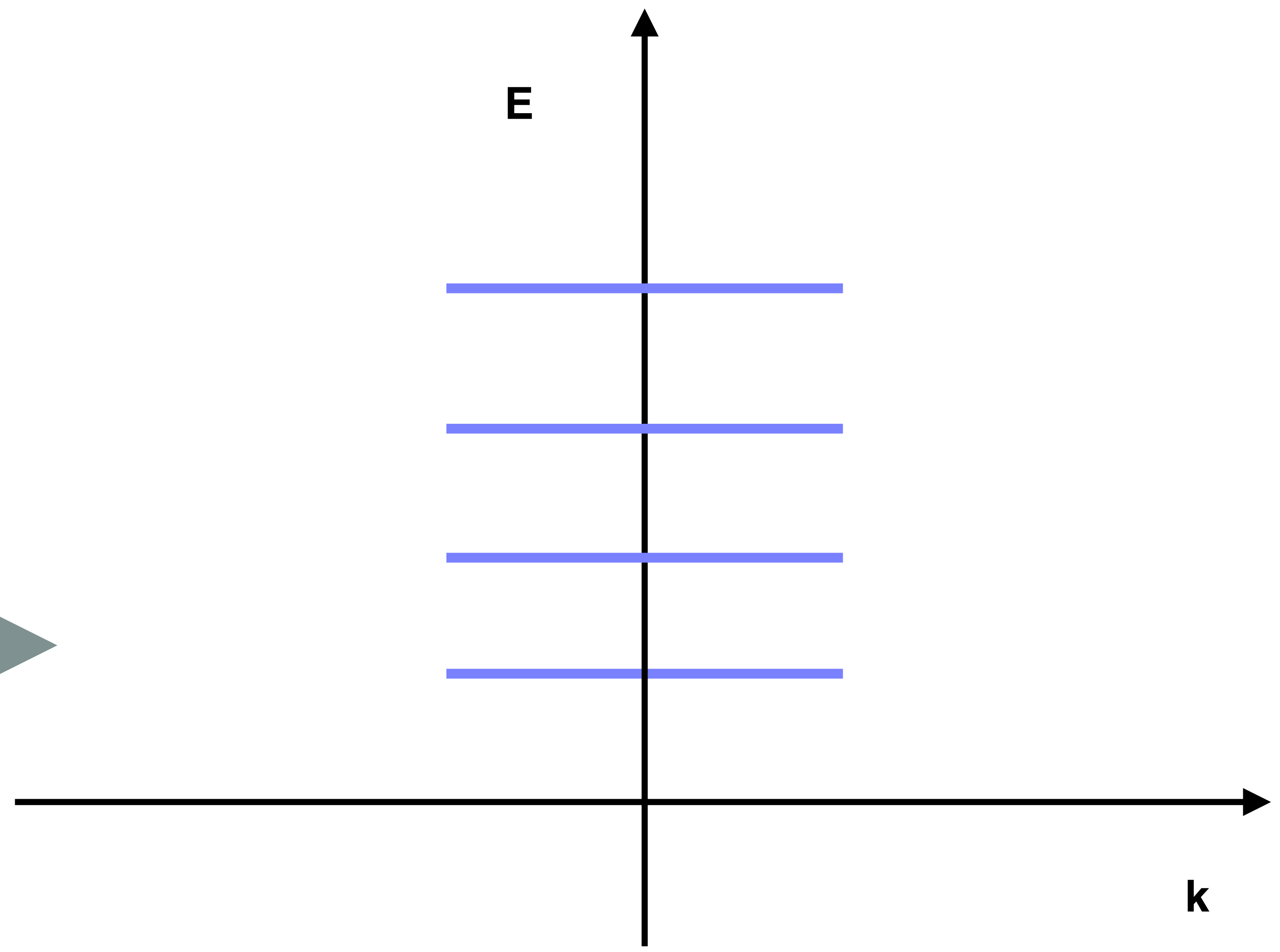


X.Hu, T.Hyart, D.Pikulin, ER. PRB(L) (2022)

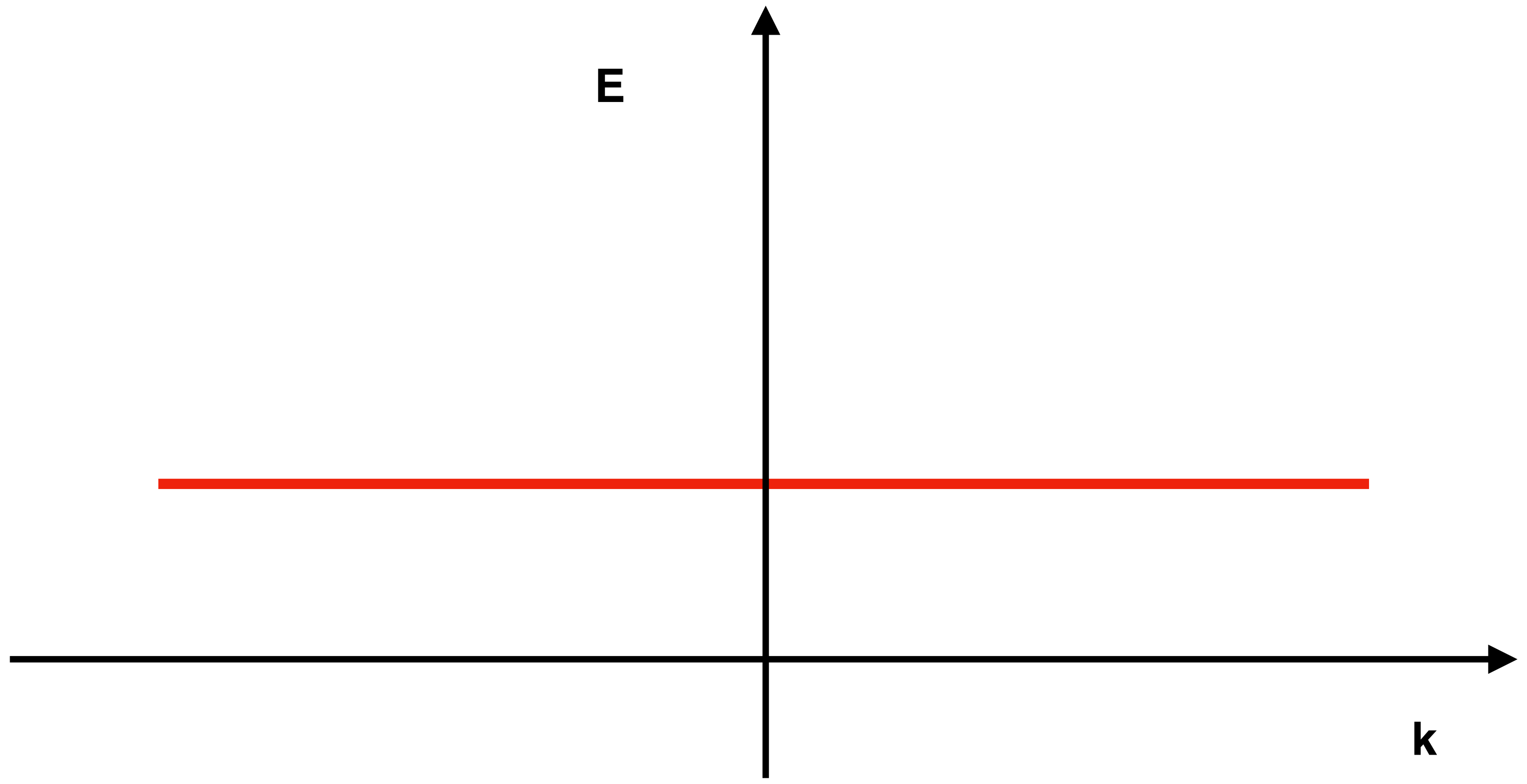
Disorder Suppression of Superfluid Stiffness. I



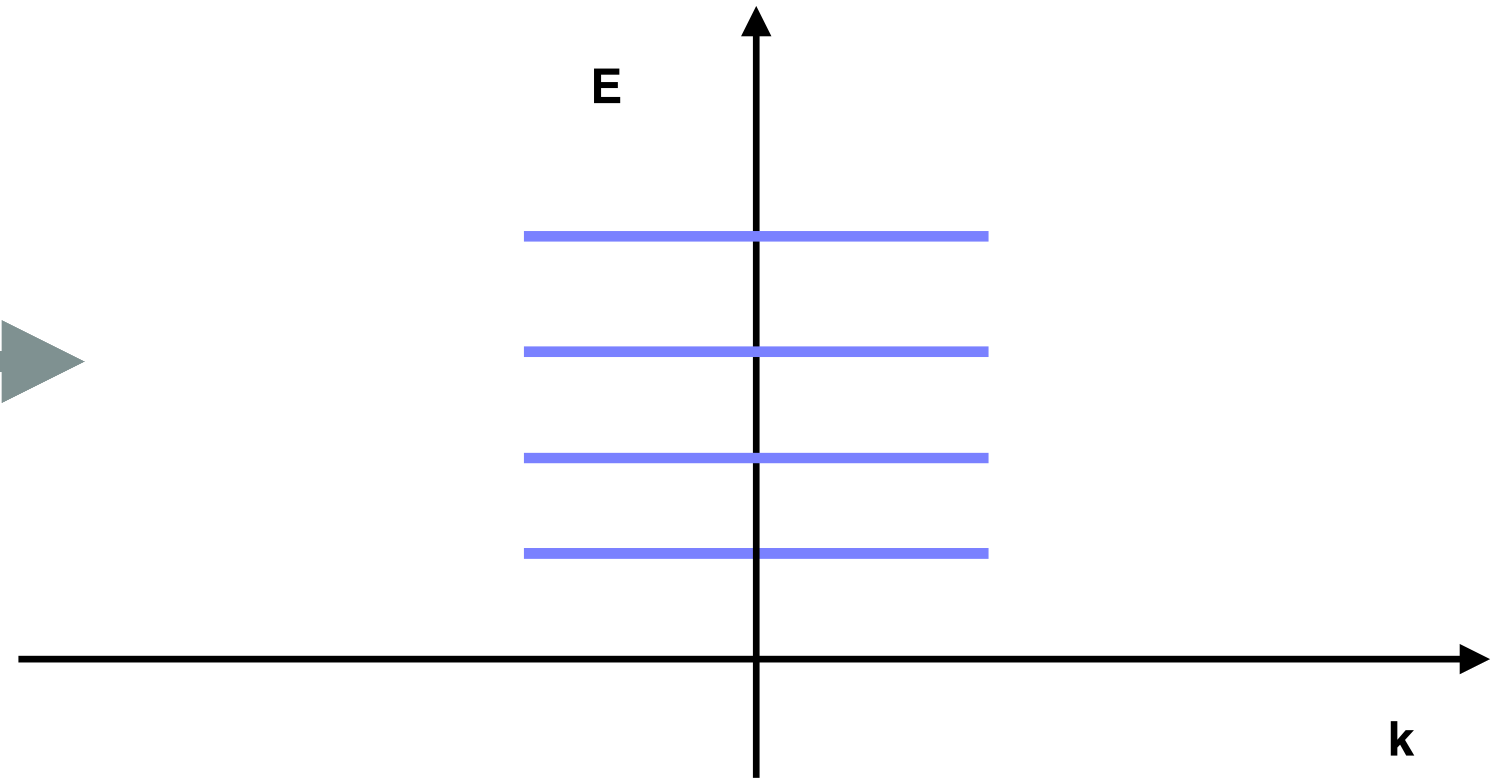
In the presence
of disorder



The disorder creates
localized bands



In the presence
of disorder



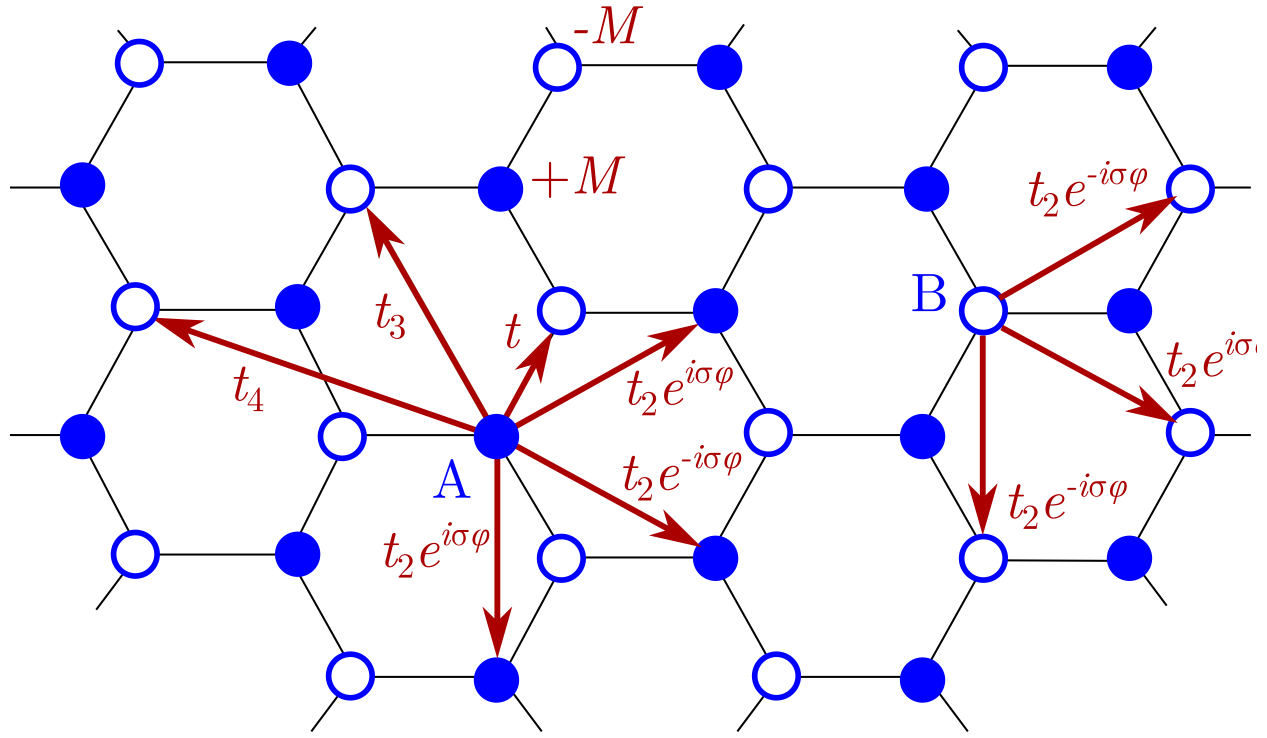
We would expect it
will impact more
the conventional
part of $D^{(s)}$

Extended Kane-Mele Model

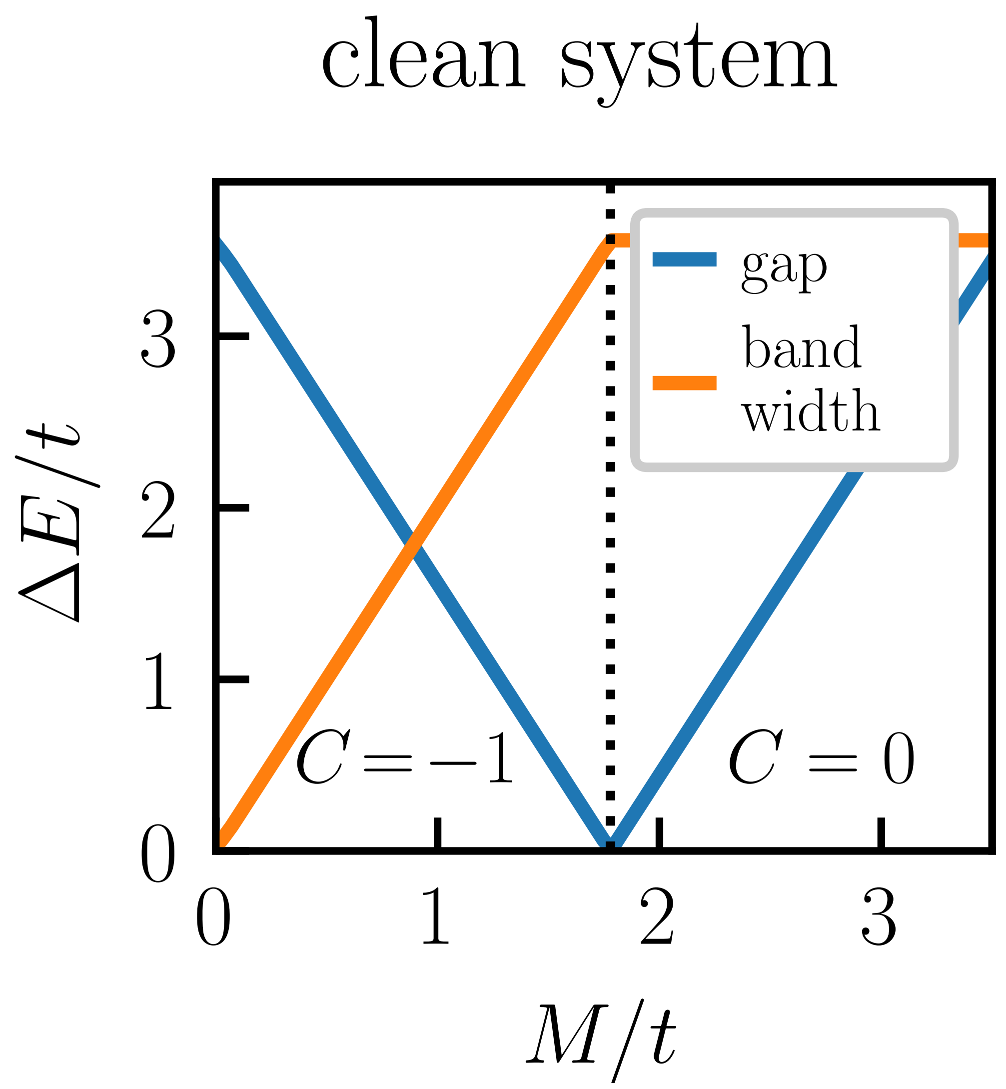
We considered an extended Kane-Mele model

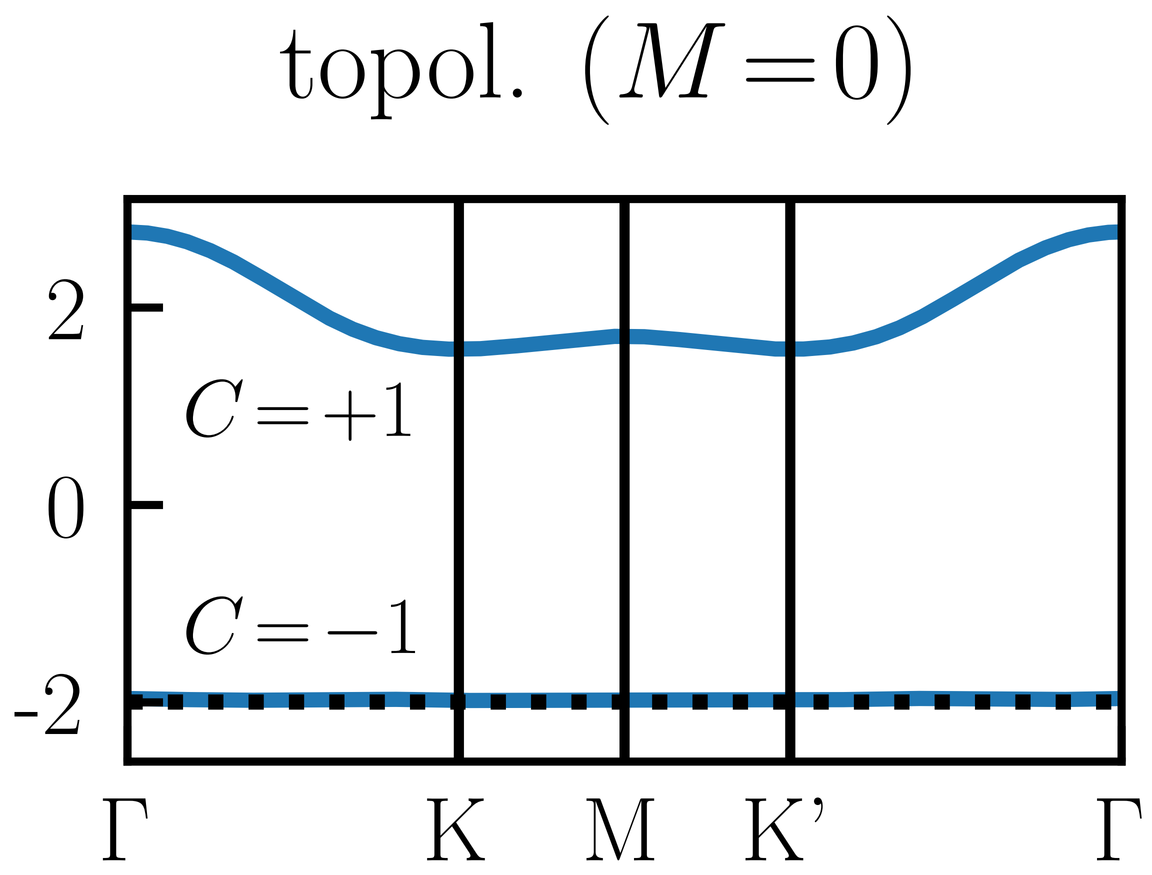
$$H_0 = \sum_{i,\sigma}\Big[(-1)^i M - \mu\Big] c^\dagger_{i\sigma} c_{i\sigma} + t\sum_{\sigma}\sum_{\langle i,j\rangle_1} c^\dagger_{j\sigma} c_{i\sigma} + t_2 \sum_{\langle i,j\rangle_2}\left(e^{i\varphi_{ij}}\, c^\dagger_{j\uparrow} c_{i\uparrow} + e^{-i\varphi_{ij}}\, c^\dagger_{j\downarrow} c_{i\downarrow}\right)$$

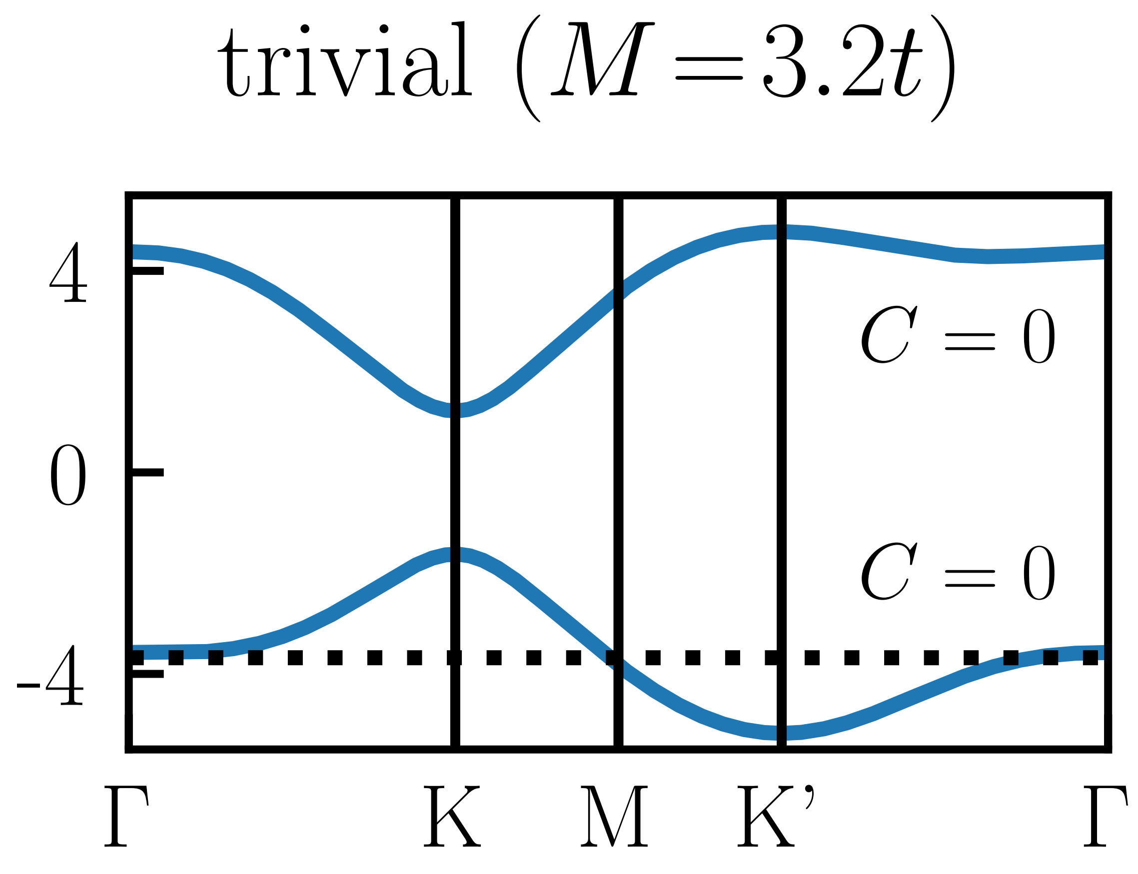
M=0 $\begin{cases} C = +1; -\pi < \varphi < 0 \\ C = -1; \quad 0 < \varphi < \pi \end{cases}$



By adding the additional hoppings t_3, t_4 w
can make the lowest energy band
extremely flat by tuning t_2, t_3 t_4, and φ



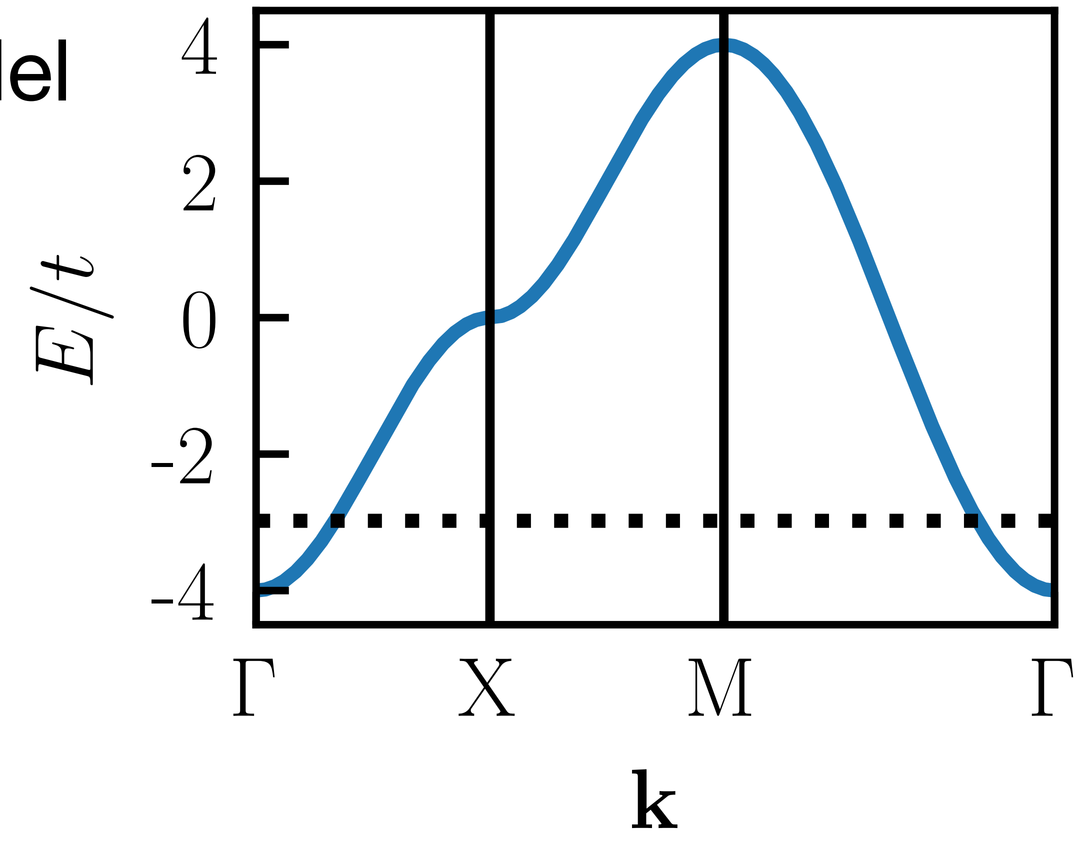




t_2=0.349 t
t_3=-0.264 t
t_4=-0.026 t
φ=1.377

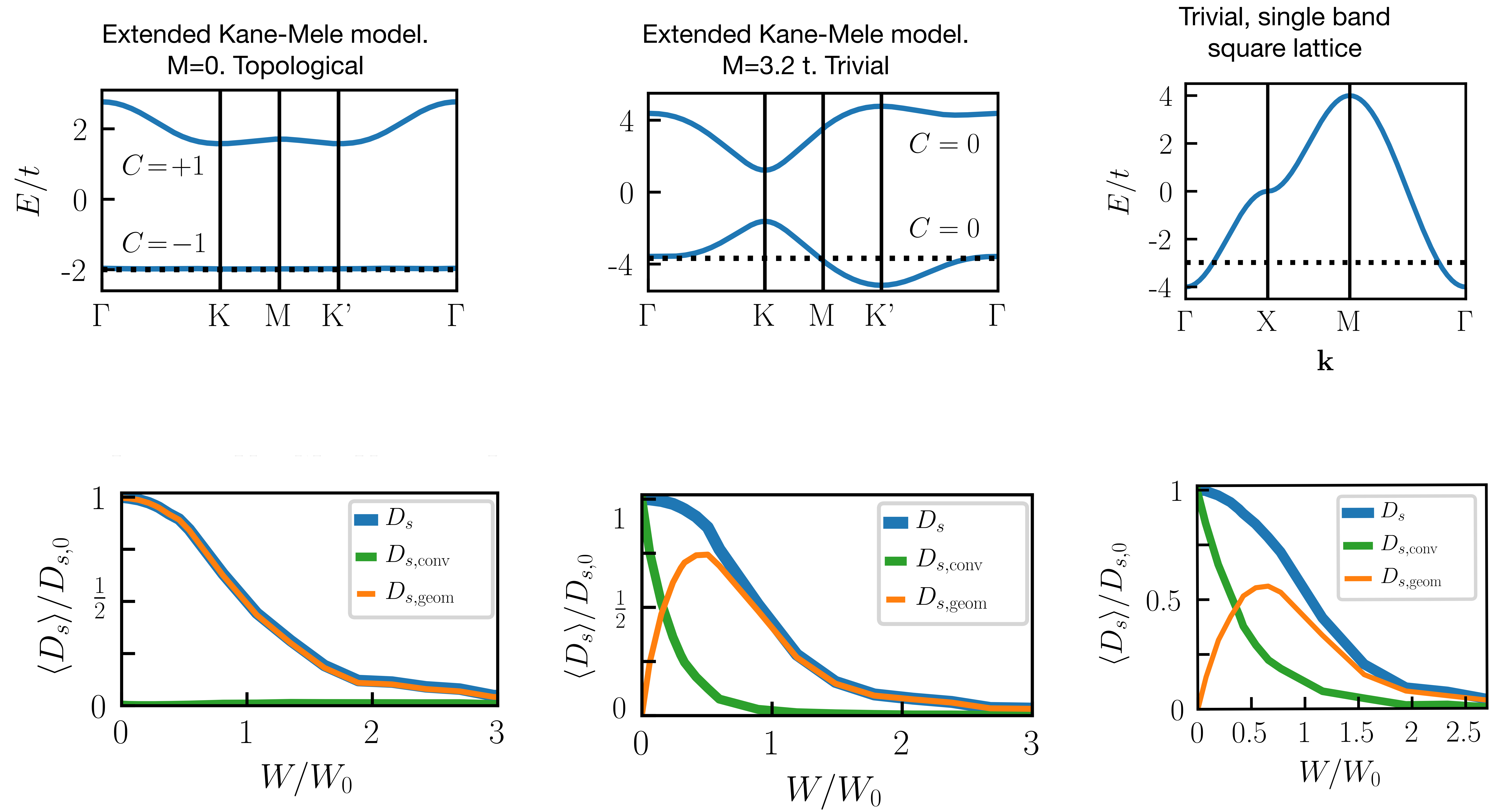
And a very trivial, single band, quadratic, model

$$H = -t\sum_{\sigma}\sum_{<i,j>} c^\dagger_{j\sigma} c_{i\sigma} - \mu \sum_{\sigma,i} c^\dagger_{i\sigma} c_{i\sigma}\,.$$



Disorder Suppression of Superfluid Stiffness. II

We consider large primitive cell with disorder and calculate self-consistently disorder-averaged superconducting gap $\langle \Delta \rangle$ and $\langle D_s \rangle$



Universal Scaling of Disorder Suppression of Superfluid Stiffness

We considered 8 different models

Extended Kane-Mele model

(i) Topological. M=0

(ii) Topological, dispersive.
M=t, $\varphi = \varphi_{\text{opt}} = 1.377$ rad.

(iii) Topological, dispersive.
M=0, $\varphi = 1.0$ rad

(iv) Close to topological transition.
M=1.75, $\varphi = \varphi_{\text{opt}}$

(v) Trivial, dispersive.
M=3.2 t, $\varphi = \varphi_{\text{opt}}$

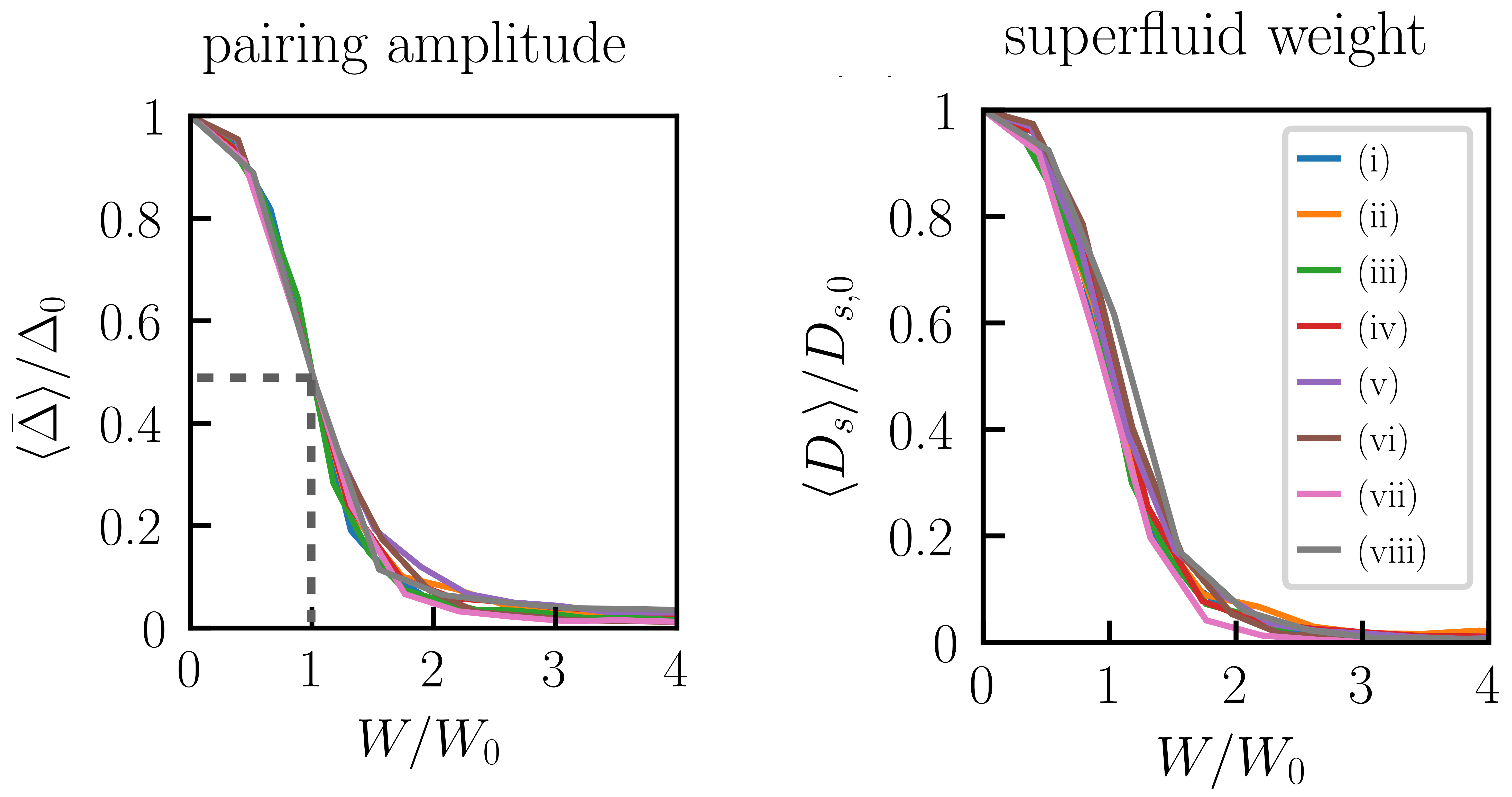
Square lattice

With parameters tuned to have in the clean limit the same $D_{s,0}$ as K-M model

(vi) t=2.0 $D_{s,0}$. U =13.4 $D_{s,0}$. Filling=1.

(vii) t=1.7 $D_{s,0}$. U =8.9 $D_{s,0}$. Filling=1.

(viii) t=3.3 $D_{s,0}$. U =13.4 $D_{s,0}$. Filling=1/5.



A. Lau et al. SciPost Physics (2022)

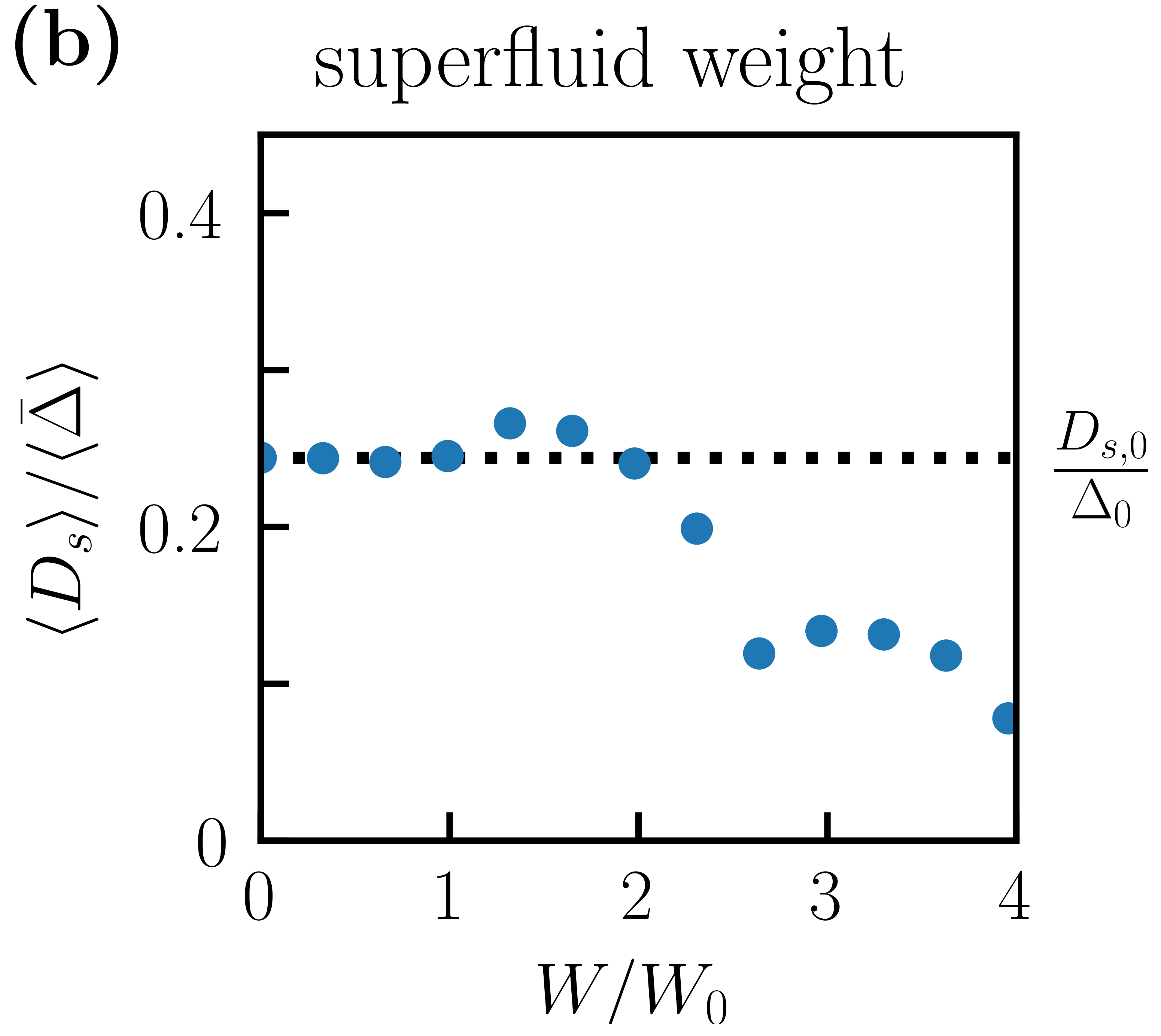
Conclusions

The real part of the Quantum Geometric Tensor $Q_{\mu\nu}$ defines a metric $g_{\mu\nu}$ for the Bloch states. Such metric can affect the properties of correlated states especially when the bands are flat. In particular:

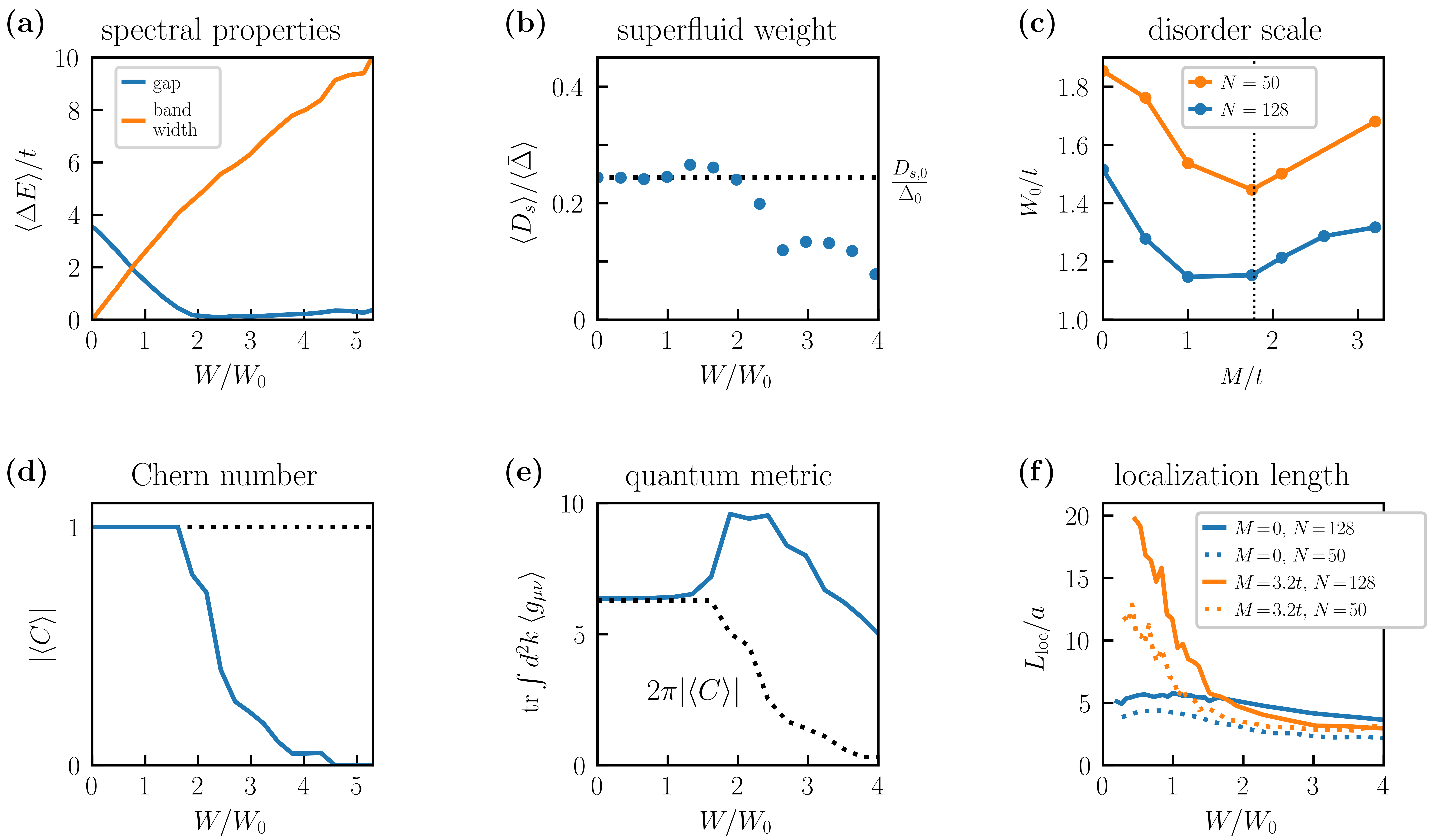
- $g_{\mu\nu}$ affects the superfluid weight (stiffness) $D^{(s)}$ of superconducting states, and more in general the stiffness of continuous order parameters
- It can explain the presence of superconductivity for multi-orbital systems even when the lowest energy band is completely flat
- For 2D superconducting states it affects T_{BKT}
- In superconducting TBLG the geometric contribution to $D^{(s)}$ dominates at the magic angle and is responsible for the unusual dependence of T_{BKT} on doping
- In double TBLG the geometric contribution to $D^{(s)}$ is essential to stabilize the exciton condensate
- The suppression with disorder of the superfluid stiffness appears to be “universal” and independent of the origin, conventional or geometric, of the stiffness

Additional Slides

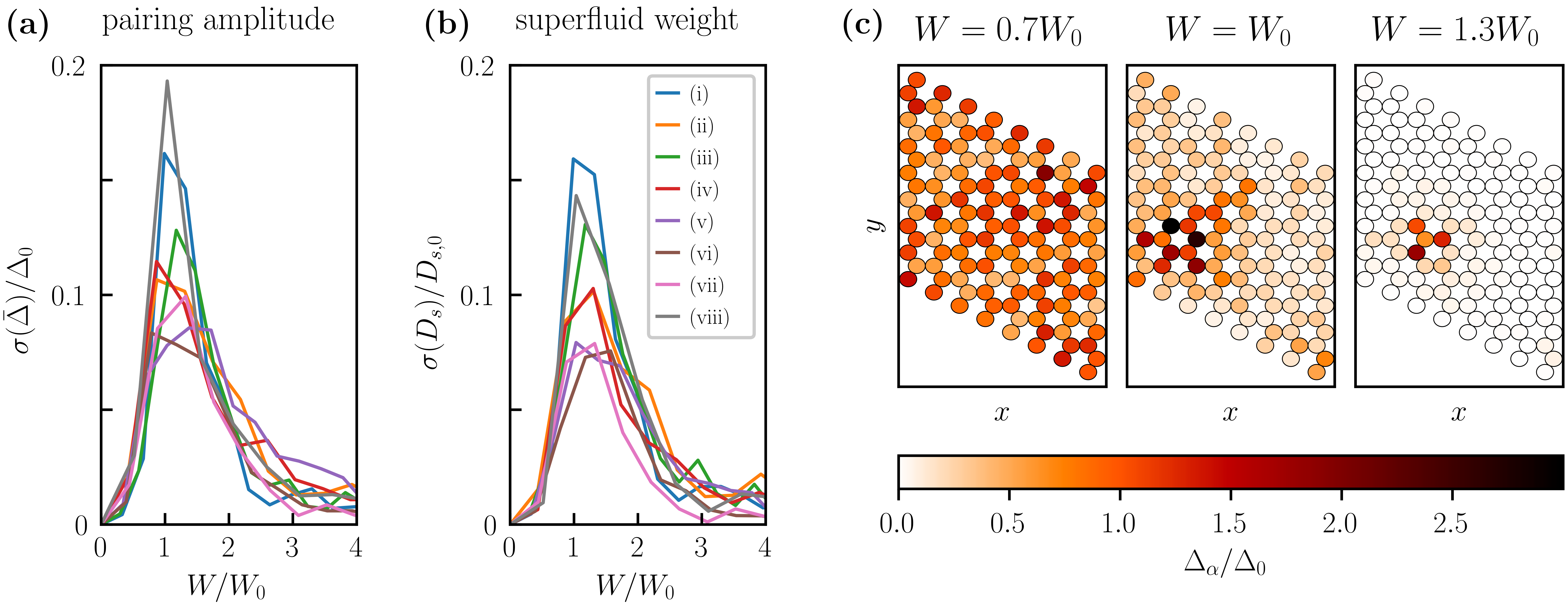
(b)


superfluid weight
$\langle D_s \rangle / \langle \bar{\Delta} \rangle$
0.4
0.2
0
0
1
2
3
4
W/W_0
$\frac{D_{s,0}}{\Delta_0}$

Additional Results for Kane-Mele Model with Optimized Flatness



Standard Deviations and Superconducting Islands



Dependence on Filling for Clean Case