Phase diagram of the two-dimensional Hubbard-Holstein model

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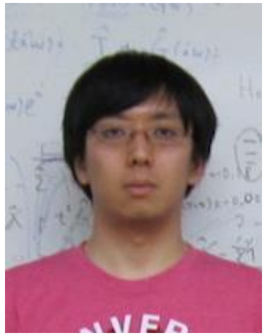
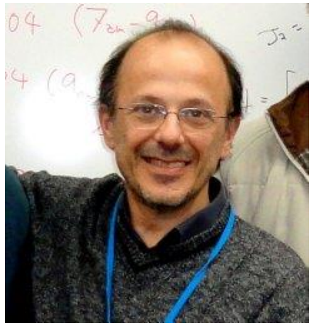
N. Costa



K. Seki

S. Yonoki



S. Sorella

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ma per seguir virtute e canoscenza
SISSA

RIKEN

Outline

- Introduction
  - Peierls Instability and CDW formation
  - Experimental motivation
- The model and methodology
- Results
  - CDW, AFM and paring in the square lattice
  - CDW and AFM in the honeycomb lattice
- Outlooks

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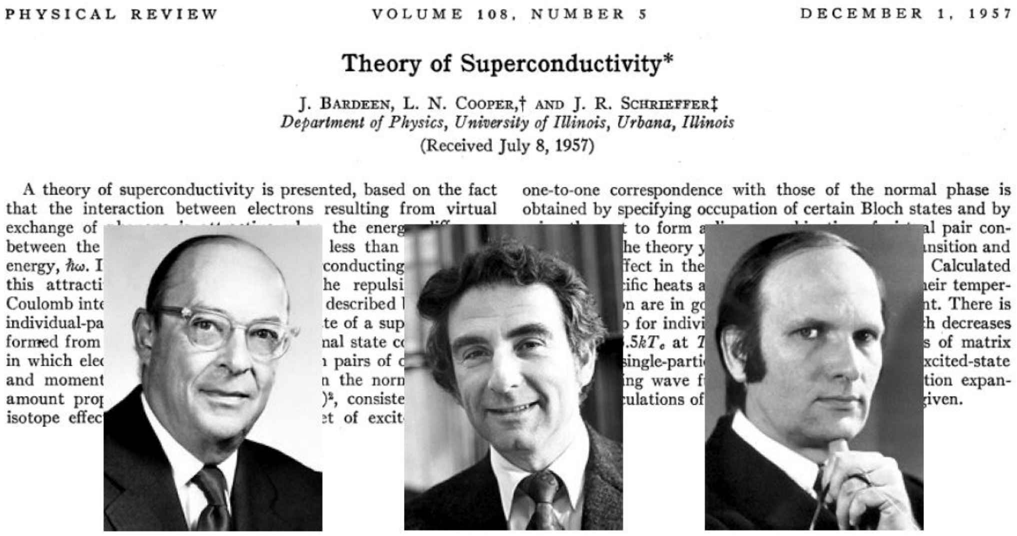
Introduction

Electron-phonon Interaction

Conventional Superconductivity



John Bardeen   Leon Neil Cooper   John Robert Schrieffer

Introduction

Electron-phonon Interaction

Conventional Superconductivity

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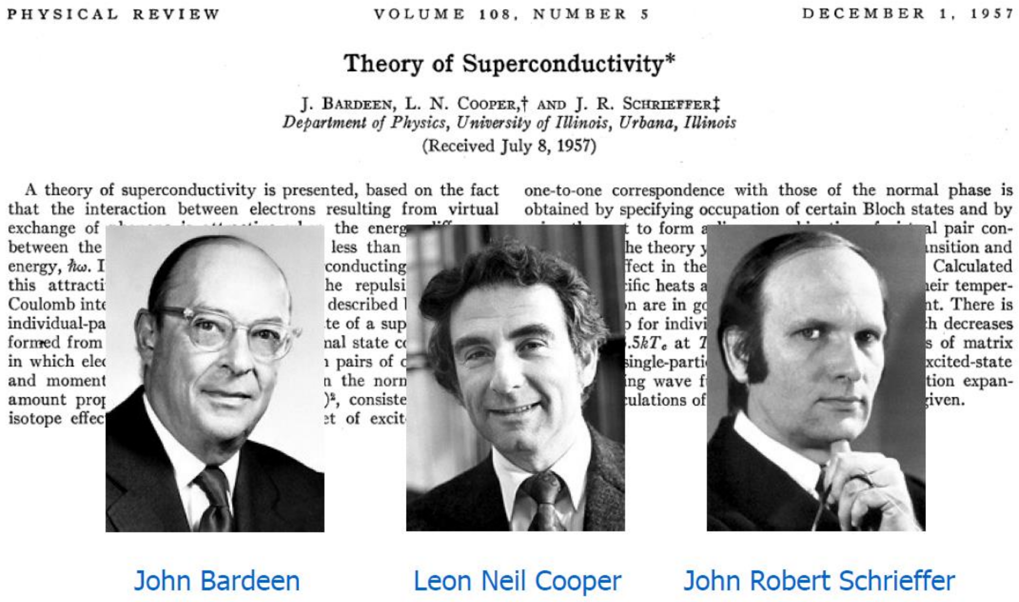
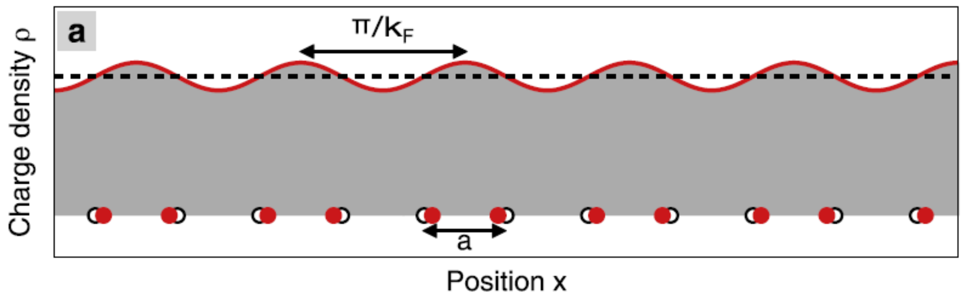
Charge modulation





Introduction

Peierls Instability → The standard explanation for charge-density wave (CDW) formation

"Recipe" for CDW …

- Fermi Surface Nesting (FSN);
- Create an electronic instability (or a lattice distortion)

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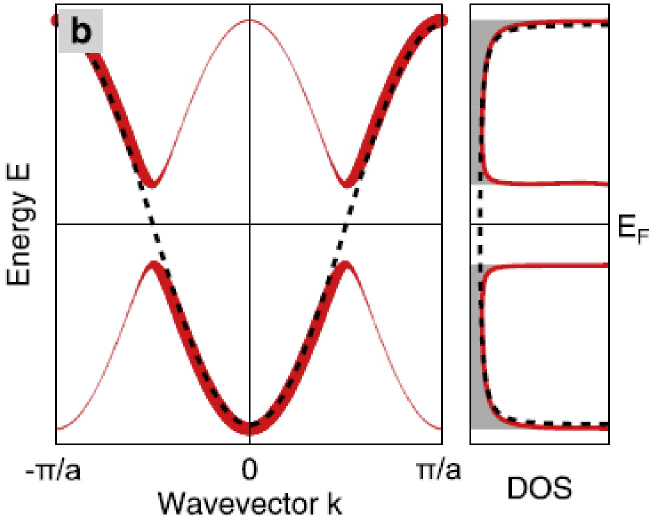
"Recipe" for CDW …

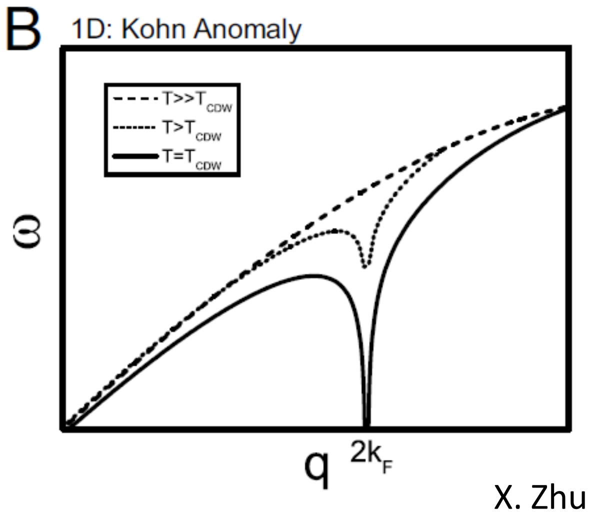
- Fermi Surface Nesting (FSN);
- Create an electronic instability (or a lattice distortion)

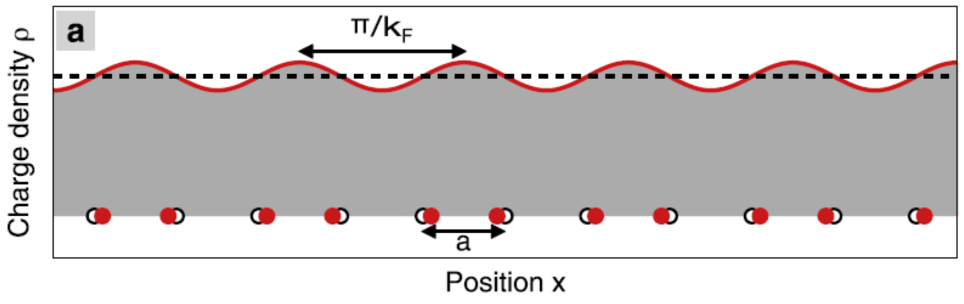
→

- Charge gap at Fermi level (metal-insulator transition);
- Phonon softening at $\mathbf{q}=2\mathbf{k}_F$;
- Permanent lattice distortion.



K. Rossnagel, J. Phys.: Condens. Matter **23** 213001 (2011)





X. Zhu et al., *Proc. Natl Acad. Sci. USA* **112**, 2367–2371 (2015)

Introduction

C.-W. Chen et al., Rep. Prog. Phys. **79** 084505 (2016)

Peierls Instability

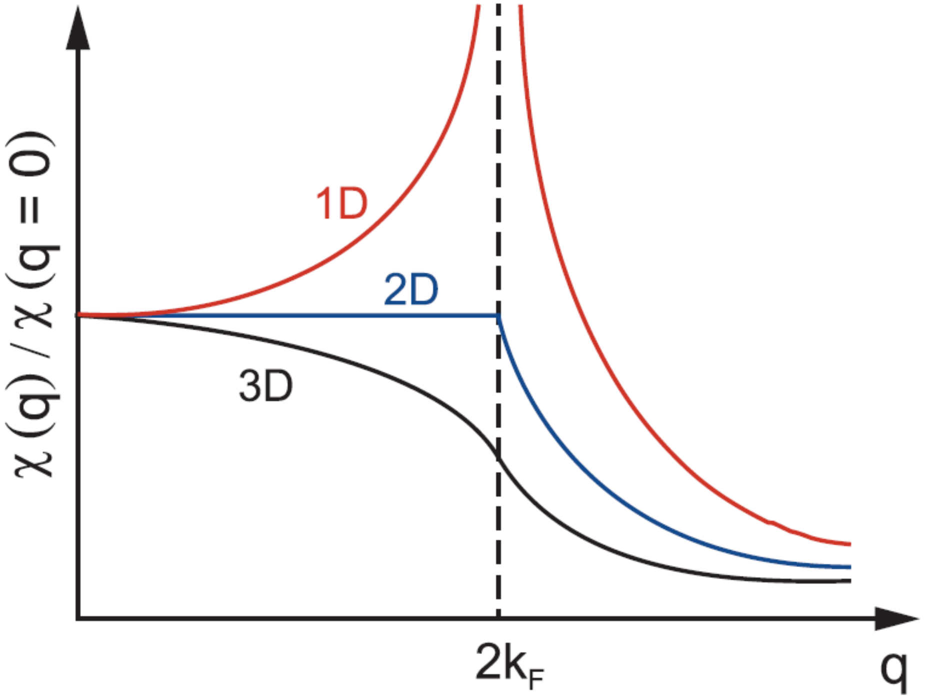
Linear Response Theory

$$\rho^{\mathrm{ind}}(\vec{r},\omega) = e^2 \int d\vec{r}'\,\chi(\vec{r},\vec{r}',\omega)\Phi^{\mathrm{tot}}(\vec{r}',\omega)$$

$$\begin{cases} \chi'(\mathbf{q}) = \sum_{\mathbf{k}} \dfrac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k+q}})}{\varepsilon_k - \varepsilon_{\mathbf{k+q}}}, \\ \lim_{\omega\to 0} \chi''(\mathbf{q},\omega)/\omega = \sum_k \delta(\varepsilon_k - \varepsilon_F)\,\delta(\varepsilon_{k+q} - \varepsilon_F) \end{cases}$$

Electronic susceptibility

Fermi gas



One-dimensional systems are highly susceptible at $\mathbf{q}=2\mathbf{k}_F$

1D: $\mathrm{Re}\chi_0 \propto -\dfrac{1}{2q}\ln\left|\dfrac{1+q/2}{1-q/2}\right|$

2D: $\mathrm{Re}\chi_0 \propto \begin{cases} -(1-\sqrt{1-(2/q)^2}), q \geq 2k_F \\ -1/E_F, q < 2k_F \end{cases}$

3D: $\mathrm{Re}\chi_0 \propto -\left[1 + \dfrac{1-(q/2)^2}{q}\ln\left|\dfrac{1+q/2}{1-q/2}\right|\right]$

Introduction

Peierls Instability

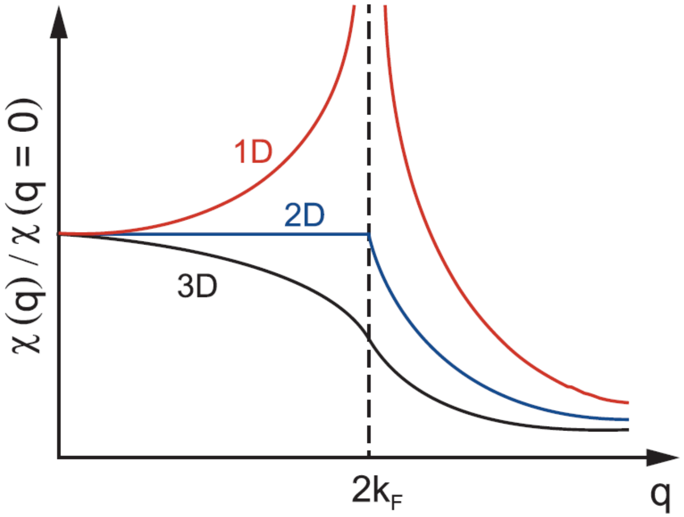
$$\phi^{\mathrm{ind}}(\mathbf{q}) = g\rho^{\mathrm{ind}}(\mathbf{q})$$

$$\rho^{\mathrm{ind}}(\mathbf{q}) = \chi_0(\mathbf{q})\phi(\mathbf{q}) = \chi_0(\mathbf{q})\left[\phi^{\mathrm{ext}}(\mathbf{q}) + \phi^{\mathrm{ind}}(\mathbf{q})\right]$$

$$\rho^{\mathrm{ind}}(\mathbf{q},T) = \frac{\chi_0(\mathbf{q},T)\phi^{\mathrm{ext}}(\mathbf{q})}{1 - g\chi_0(\mathbf{q},T)} \qquad 1 - g\chi_0(\mathbf{q},T) = 0$$

Fröhlich Hamiltonian

$$H_{\mathrm{PI}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a^{+}_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} b^{+}_{\mathbf{q}} b_{\mathbf{q}} + \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} g_{\mathbf{q}} a^{+}_{\mathbf{k}+\mathbf{q}} a_{\mathbf{k}} (b^{+}_{-\mathbf{q}} + b_{\mathbf{q}}),$$



C.-W. Chen et al., Rep. Prog. Phys. **79** 084505 (2016)

For ideal 1D systems *any* Electron-Phonon Coupling leads to CDW!

Criterion to CDW (Perturbation theory)

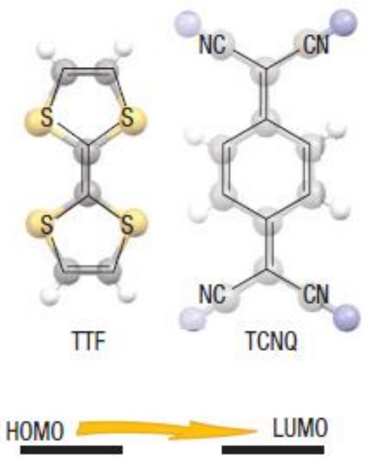
$$\frac{4g^2_{\mathbf{q}}}{\hbar\omega_{\mathbf{q}}} > \frac{1}{\chi_0(\mathbf{q})}$$

More generally

$$\frac{4g^2_{\mathbf{q}}}{\hbar\omega_{\mathbf{q}}} - 2U_{\mathbf{q}} + V_{\mathbf{q}} \geqslant \frac{1}{\chi_0(\mathbf{q})}$$

Introduction

Organic molecular crystal
tetrathiafulvalene-tetracyanoquinodimethane
(TTF-TCNQ)



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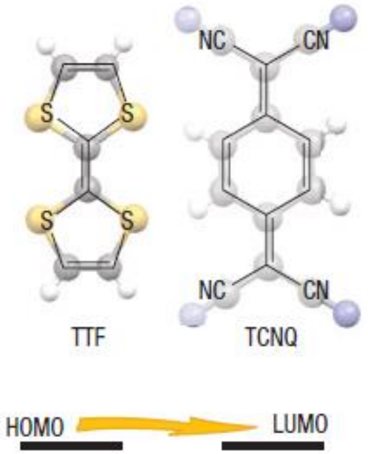
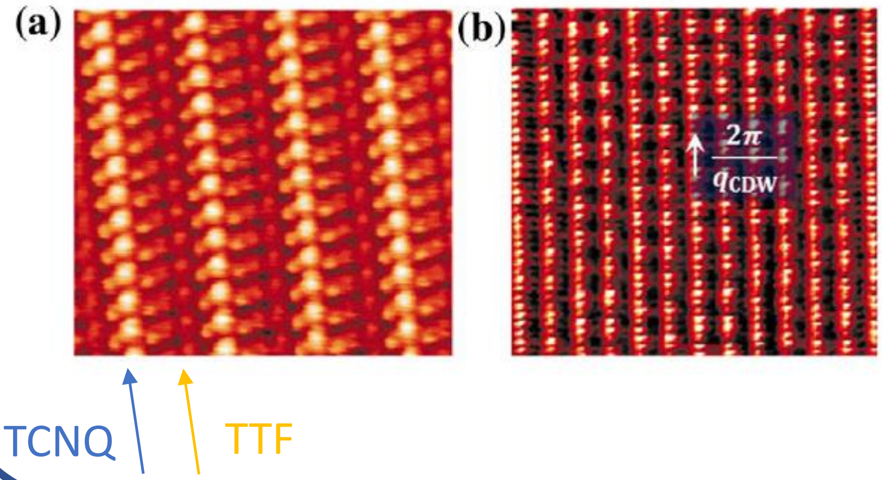


STM measurements

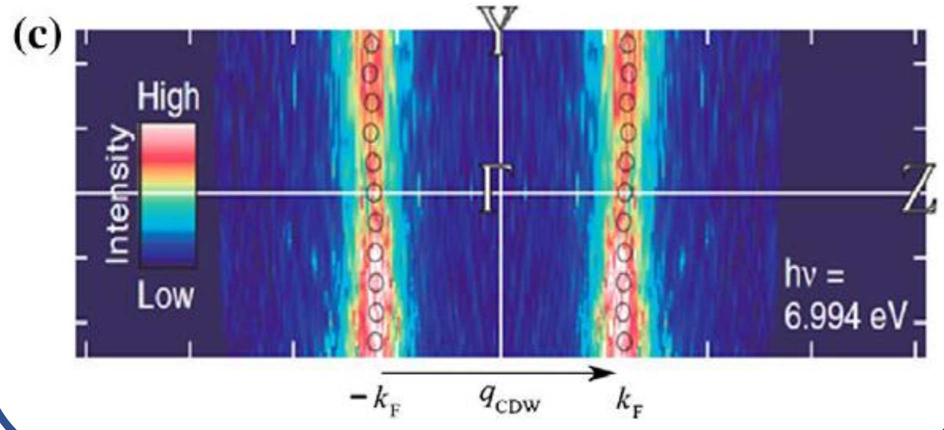
63 K (normal state)

36 K (CDW state)



ARPES measurements

60 K (normal state)



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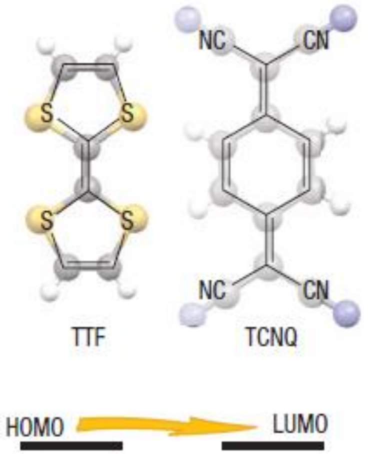

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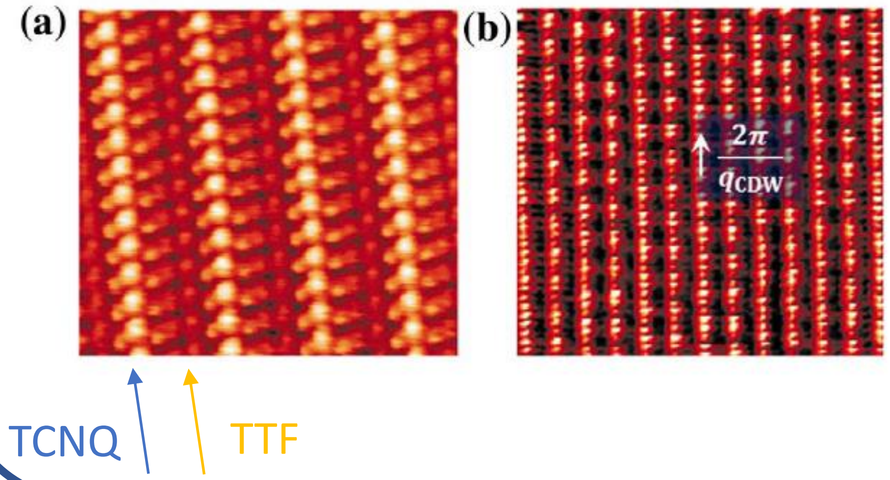
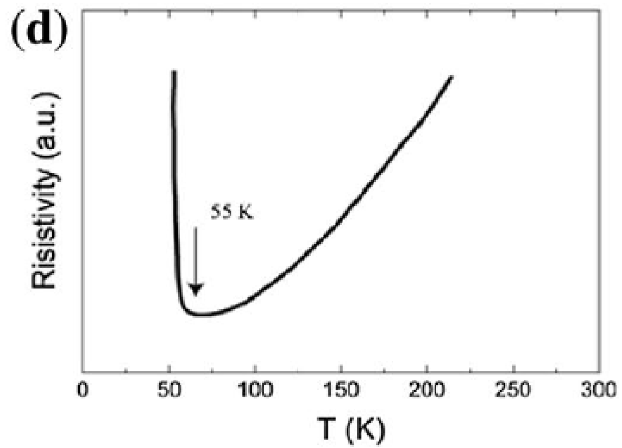
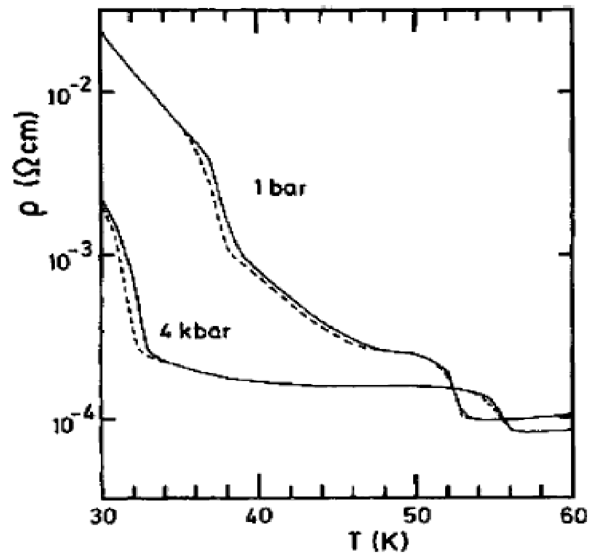
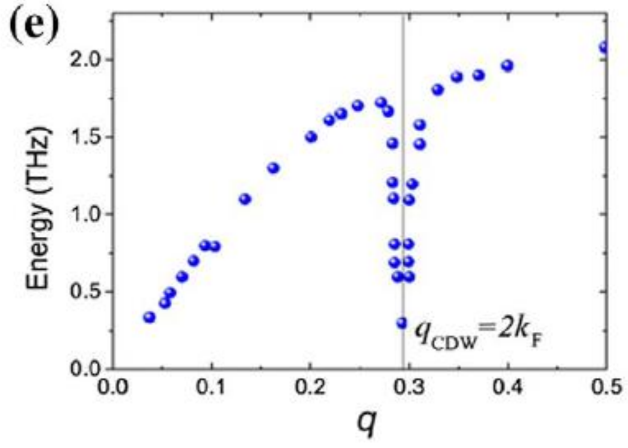


Resistivity





Inelastic neutron scattering



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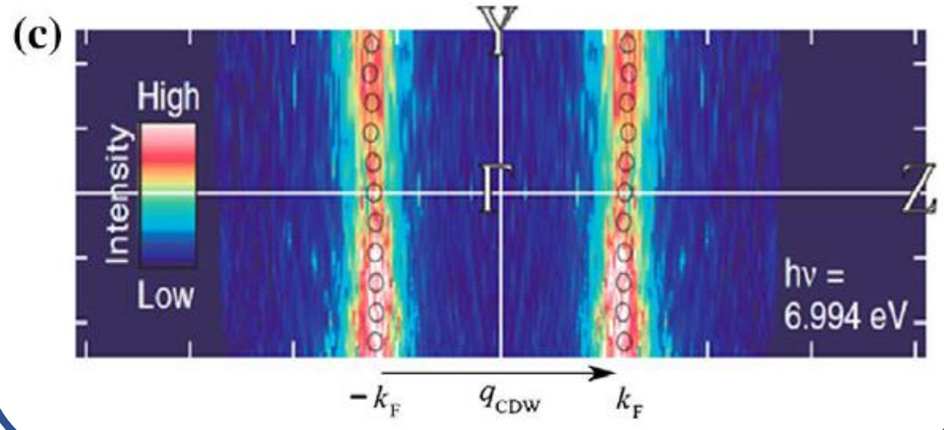

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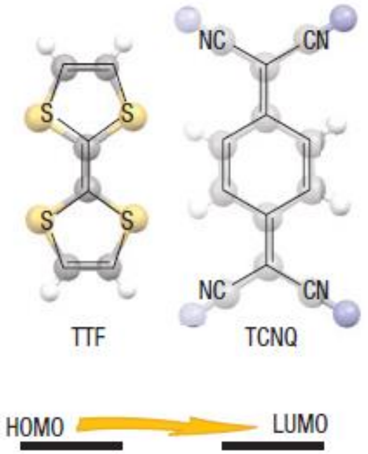

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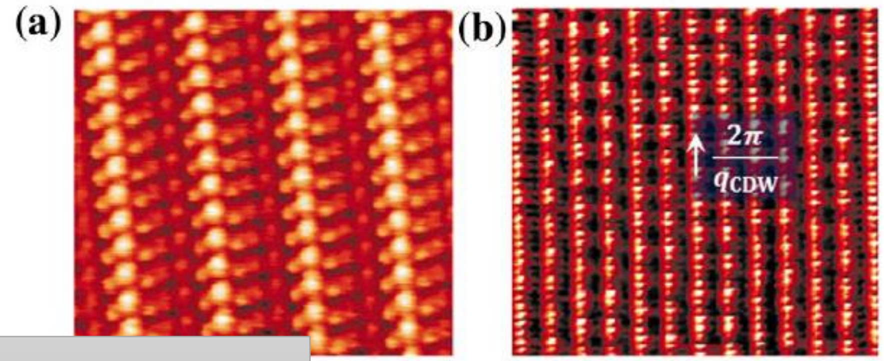

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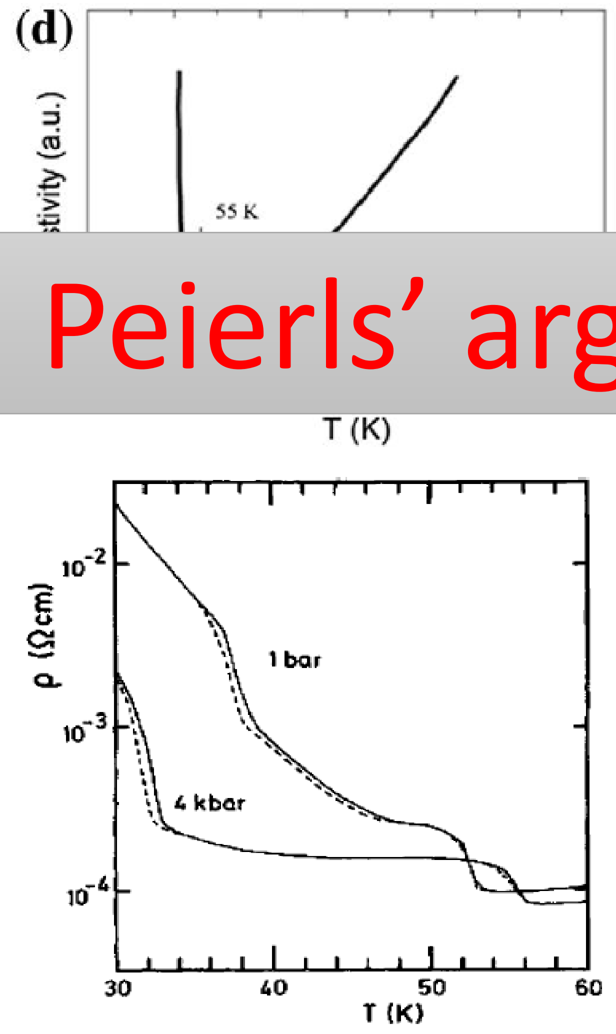

✓ Peierls' argument

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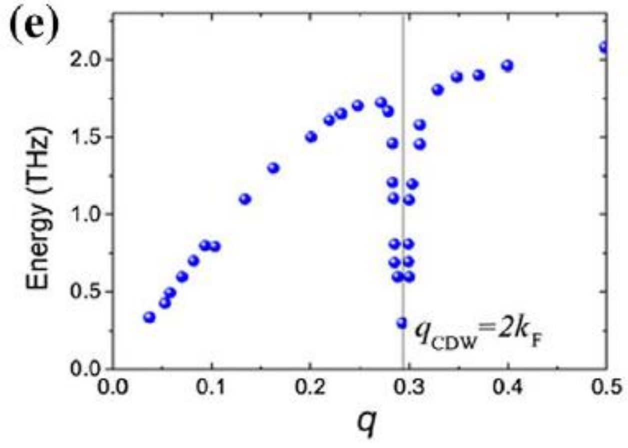

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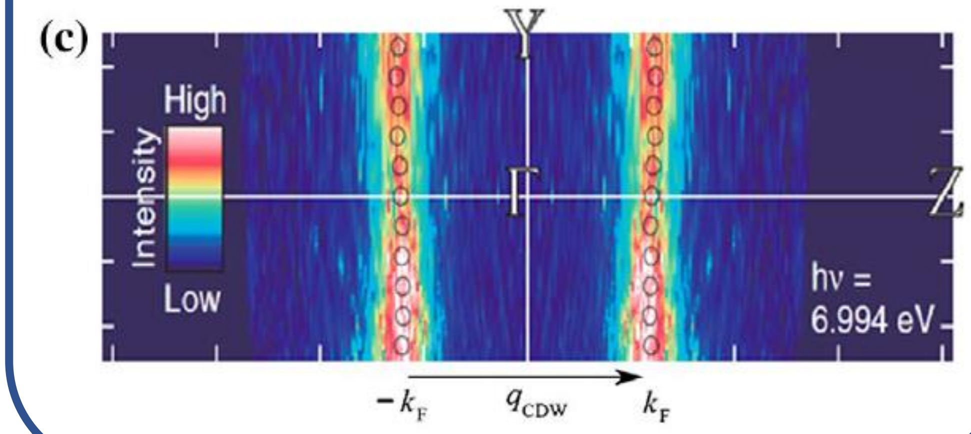
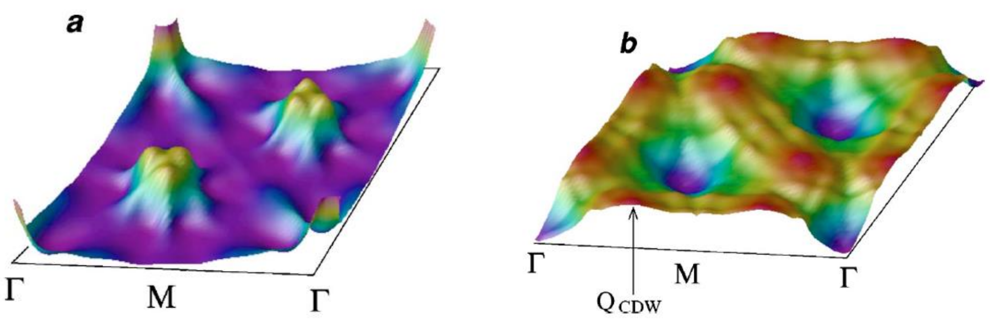


Introduction

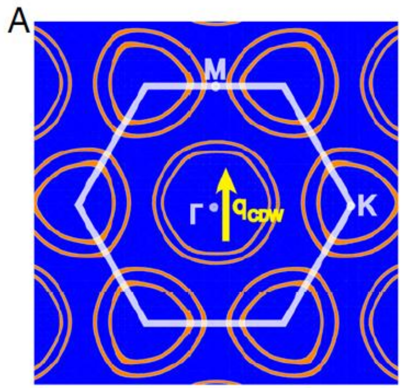
The Nature of CDW

NbSe₂ → Quasi-2D material



$\lim_{\omega \to 0} \chi''(\mathbf{q},\omega)/\omega$ $\chi'(\mathbf{q})$

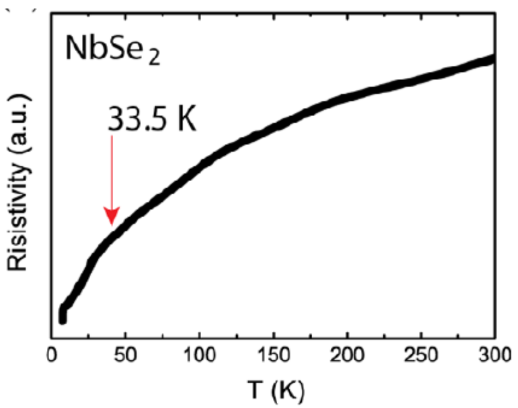
M. D. Johannes, I. I. Mazin, and C. A. Howells, Phys. Rev. B **73**, 205102 (2006).



X. Zhu et al., *Proc. Natl Acad. Sci. USA* **112**, 2367–2371 (2015)

- No electronic divergence
- No FSN
- No metal-insulator transition

CDW at $q_{CDW} = (2/3)|\Gamma M|$



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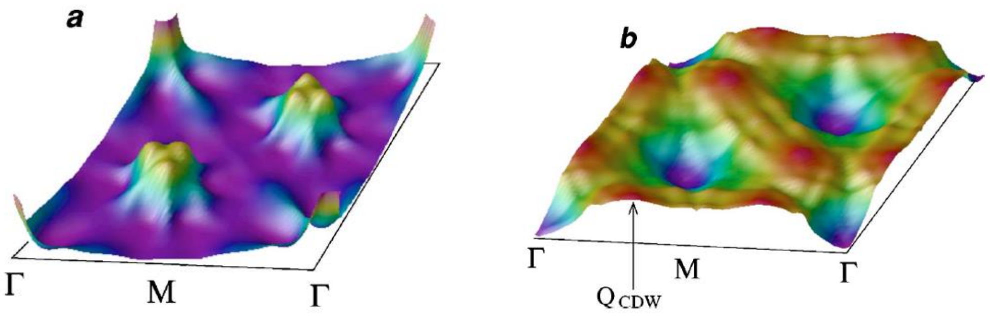
Introduction

The Nature of CDW | $NbSe_2$ → Quasi-2D material



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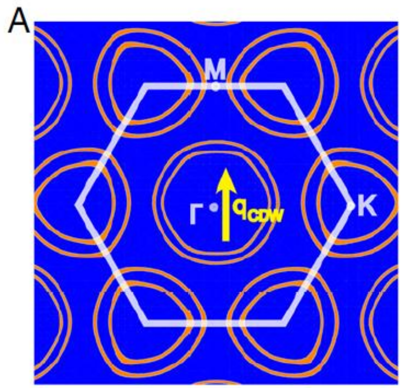

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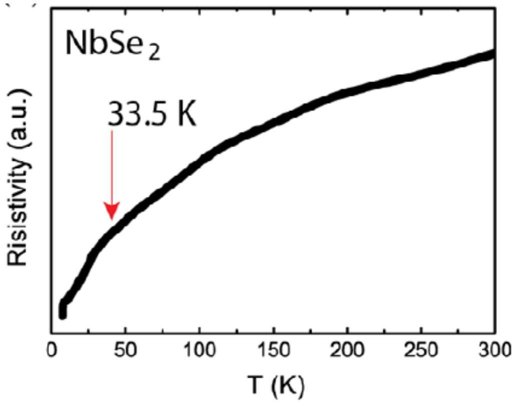

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✘ ~~Peierls' argument~~

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The Nature of CDW

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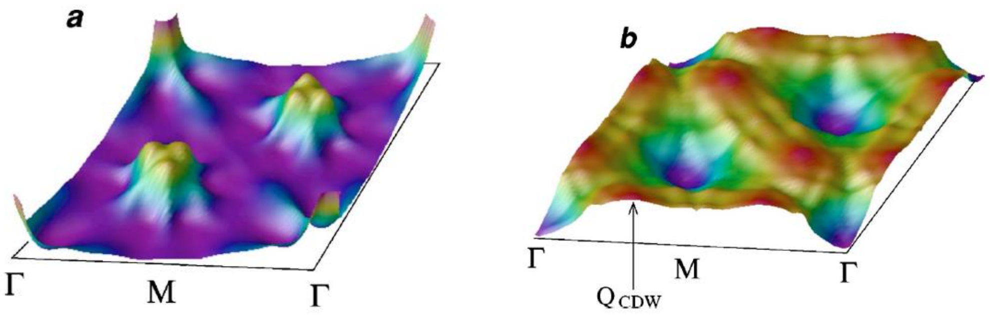

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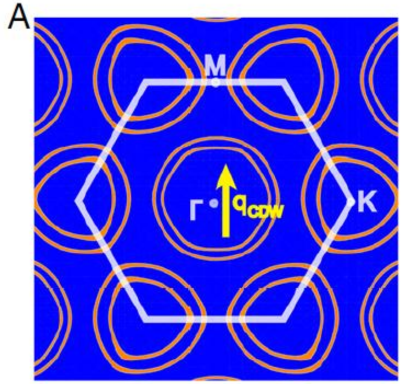

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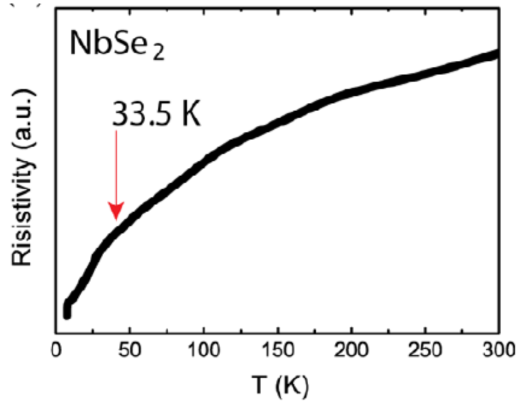

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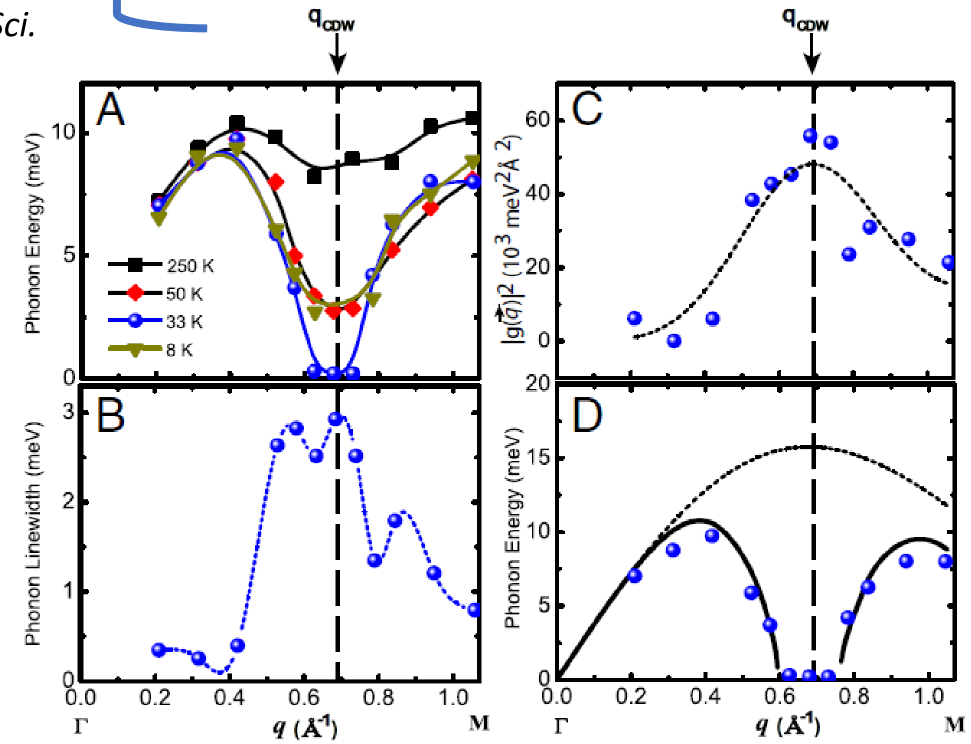
$$\Gamma_{EPC}(\vec{q}) = -2|g(\vec{q})|^2 \ \mathrm{Im}[\chi(\omega,\vec{q})]$$

Measurements of phonon linewidth provide a direct measurement of EPC.



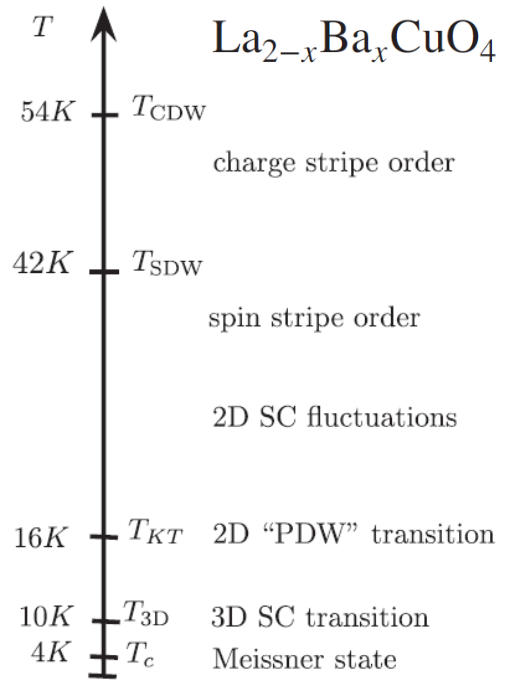
Strong Evidence of a (non-Peierls) CDW by EPC

Introduction

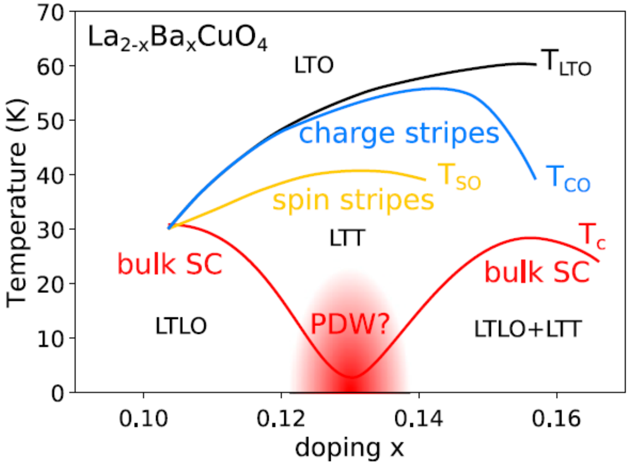
Cuprates

Introduction

E. Fradkin et al, RMP **87**, 457 (2015)

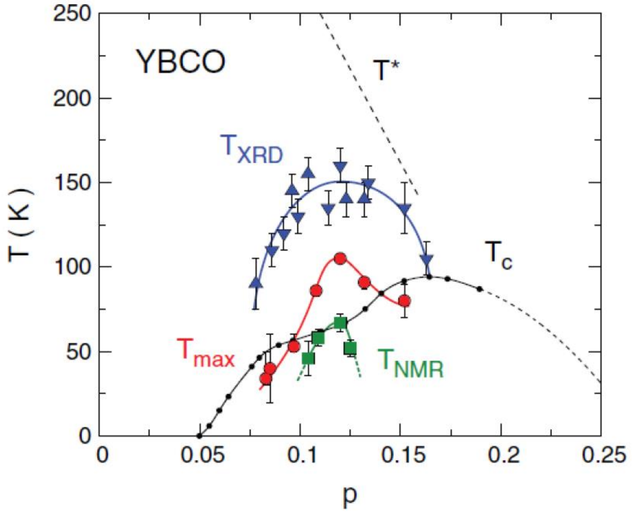


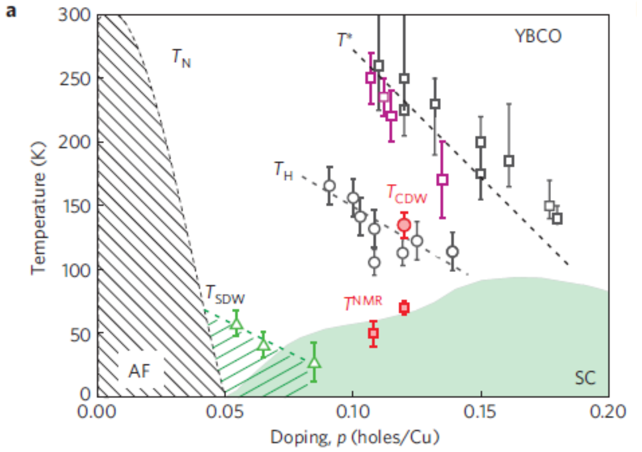
M. Leroux et al, PNAS **116**, 10691 (2018)



Cuprates

Cyr-Choiniere, et. al, Phys. Rev. B 98, 064513 (2018)





J. Chang et al, Nat. Phys. **8**, 871 (2012).

Introduction

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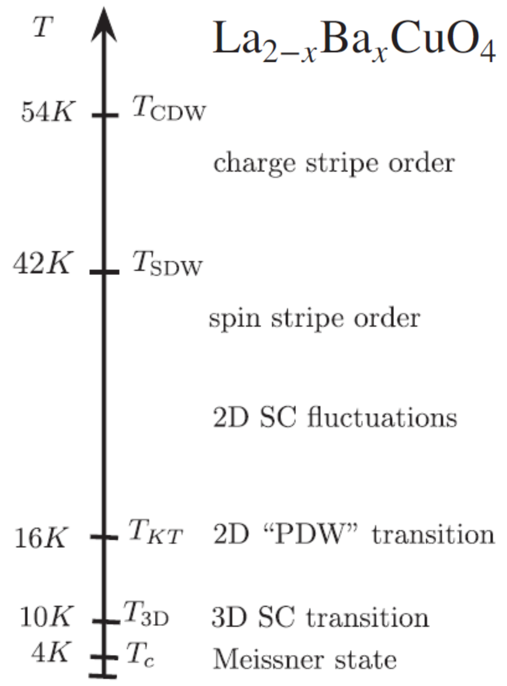

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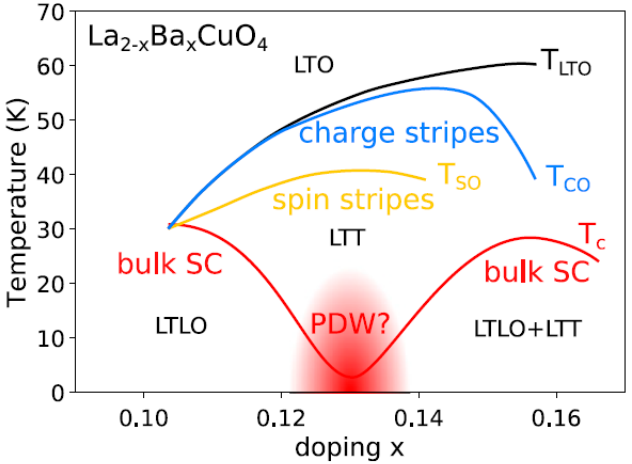

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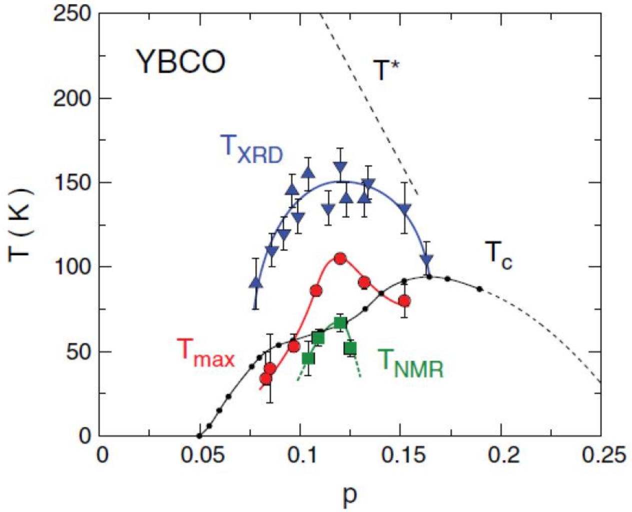

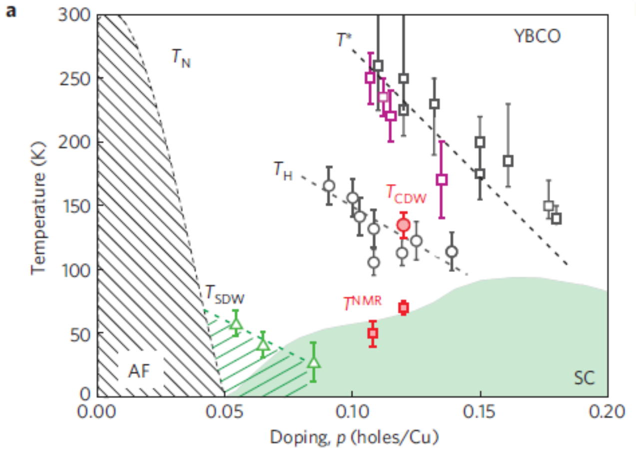

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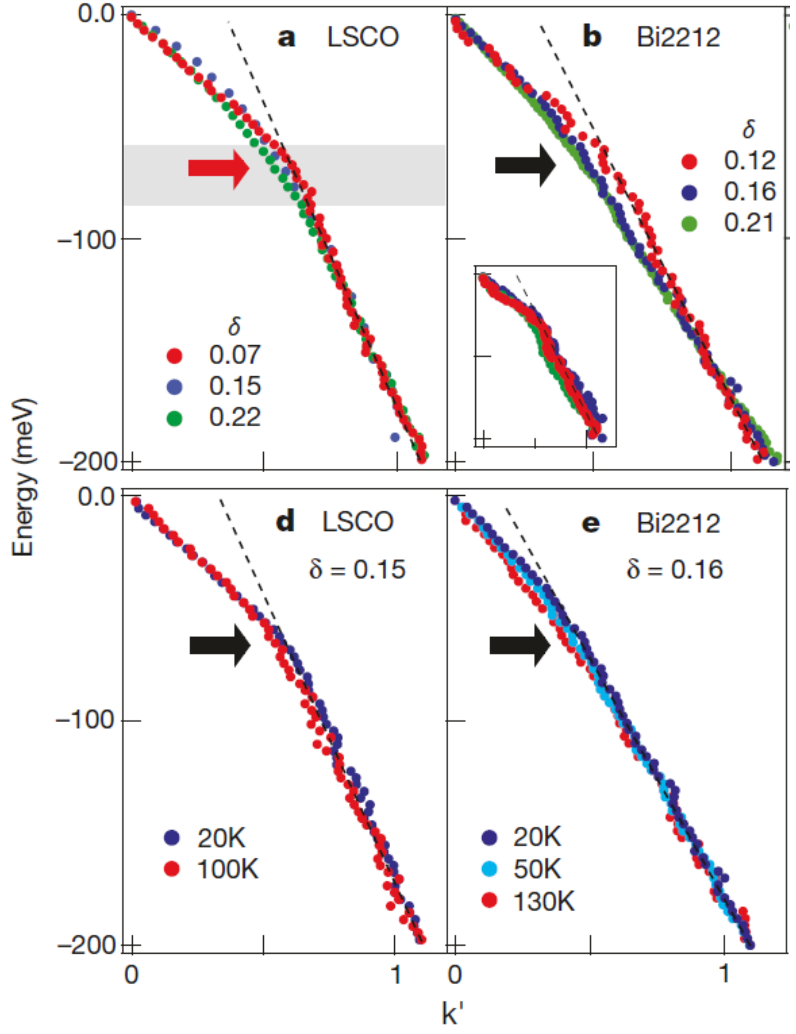
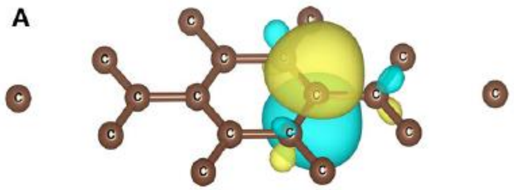


A. Lanzara et al, Nature **412**, 510 (2001)

Introduction

Graphene



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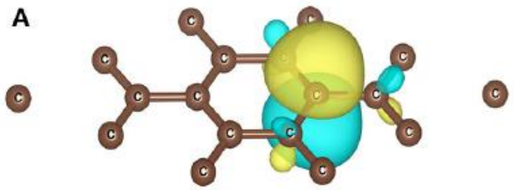
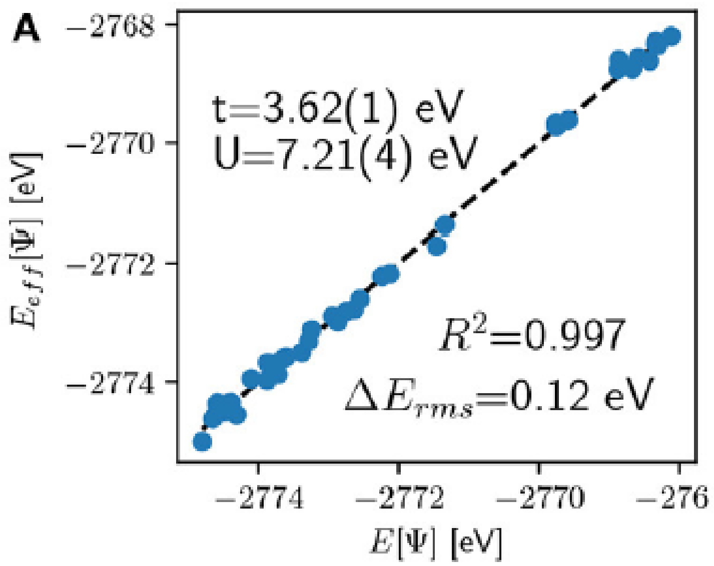


H. Zheng et al, Frontiers in Physics 6, 43 (2018)



Determination of the *e-e* interactions: ab-initio + strongly correlated methods

PRL **106,** 236805 (2011) PHYSICAL REVIEW LETTERS week ending 10 JUNE 2011

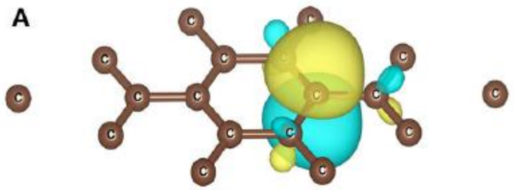
Strength of Effective Coulomb Interactions in Graphene and Graphite

T. O. Wehling,[1] E. Şaşıoğlu,[2] C. Friedrich,[2] A. I. Lichtenstein,[1] M. I. Katsnelson,[3] and S. Blügel[2]
[1]*Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany*
[2]*Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany*
[3]*Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands*
(Received 25 January 2011; published 8 June 2011)

$U_{00} = 9.3$ eV $\qquad U_{01} = 5.5$ eV $\qquad t \approx 2.8$ eV

Introduction

Graphene



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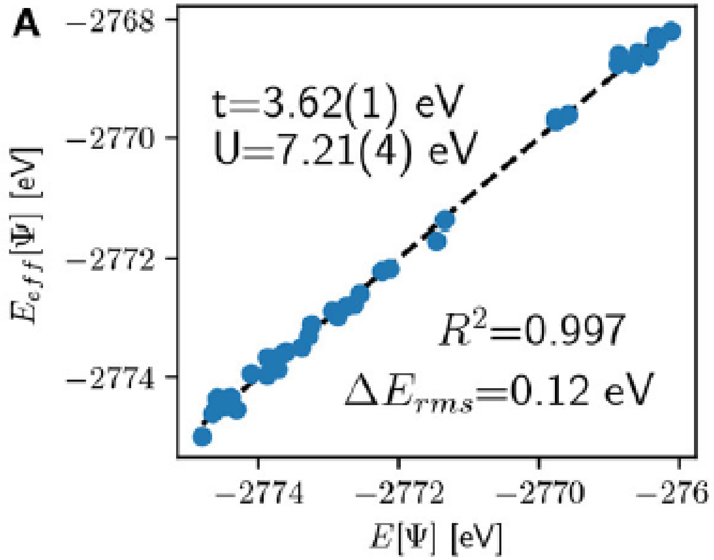


Determination of the *e-e* interactions: ab-initio + strongly correlated methods

$U_{eff}/t < 3.8$

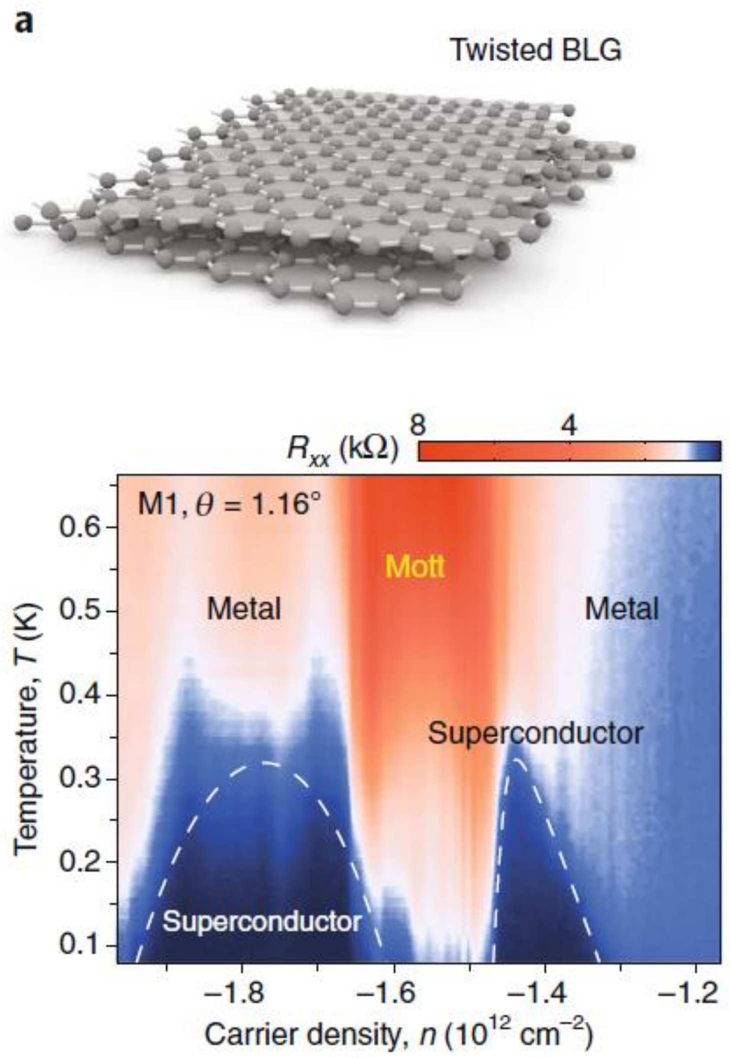
QCP for the metal-insulator transition in the honeycomb lattice

PRL **106,** 236805 (2011) PHYSICAL REVIEW LETTERS week ending 10 JUNE 2011

Strength of Effective Coulomb Interactions in Graphene and Graphite

T. O. Wehling,[1] E. Şaşıoğlu,[2] C. Friedrich,[2] A. I. Lichtenstein,[1] M. I. Katsnelson,[3] and S. Blügel[2]
[1]*Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany*
[2]*Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany*
[3]*Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands*
(Received 25 January 2011; published 8 June 2011)

$U_{00} = 9.3$ eV $\quad U_{01} = 5.5$ eV $\quad t \approx 2.8$ eV



L. Balents et al, Nature Physics **16**, 725 (2020)

PHYSICAL REVIEW LETTERS **122,** 257002 (2019)

Twisted Bilayer Graphene: A Phonon-Driven Superconductor

Biao Lian,[1] Zhijun Wang,[2,3] and B. Andrei Bernevig[4,5,6]
[1]*Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA*
[2]*Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
[3]*University of Chinese Academy of Sciences, Beijing 100049, China*
[4]*Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*
[5]*Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universitat Berlin, Arnimallee 14, 14195 Berlin, Germany*
[6]*Max Planck Institute of Microstructure Physics, 06120 Halle, Germany*

PHYSICAL REVIEW LETTERS **121,** 257001 (2018)

Theory of Phonon-Mediated Superconductivity in Twisted Bilayer Graphene

Fengcheng Wu,[1,2] A. H. MacDonald,[3] and Ivar Martin[1]
[1]*Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
[2]*Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, Maryland 20742, USA*
[3]*Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA*

Introduction

How the EPI affects the properties of SCES?

- Occurrence of long-range order
  - AFM
  - Charge ordering
  - Superconductivity

Introduction

How the EPI affects the properties of SCES?

- Occurrence of long-range order
  - AFM
  - Charge ordering
  - Superconductivity

- Most of the works are at 1D;
- Most of the works for D>1 use biased methodologies

We performed unbiased zero and finite temperature auxiliary-field QMC simulations in 2D lattices (square and honeycomb) for an effective lattice Hamiltonian that takes into account both e-e and e-ph interactions:

The Hubbard-Holstein model.

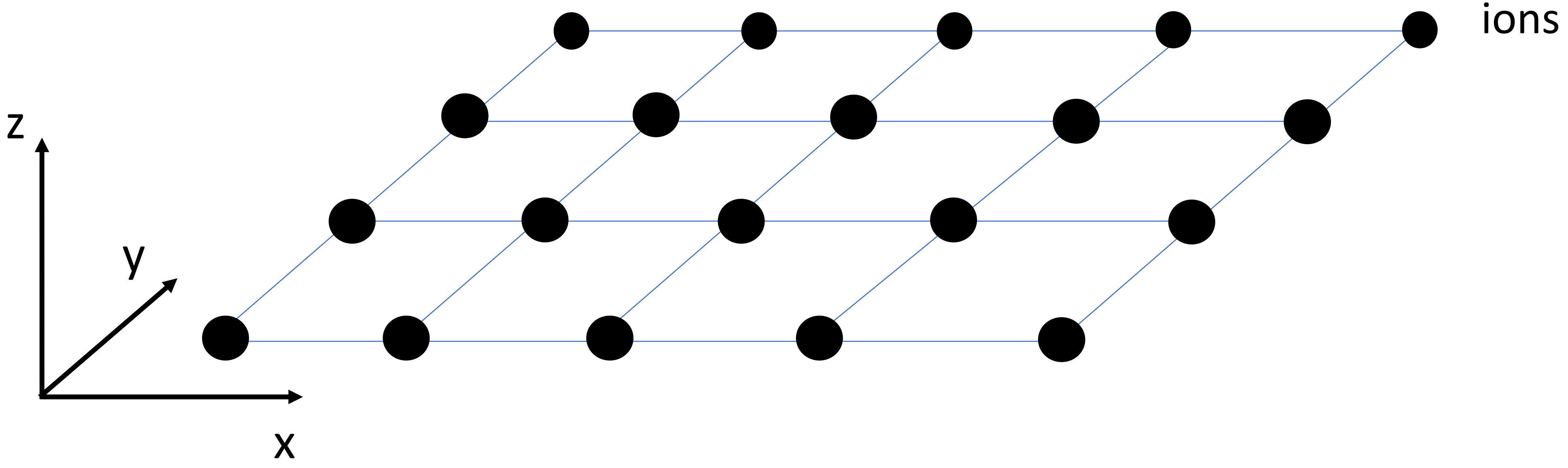
Outline

- Introduction
  - Peierls Instability and CDW formation
  - Experimental motivation
- The model and methodology
- Results
  - CDW, AFM and paring in the square lattice
  - CDW and AFM in the honeycomb lattice
- Outlooks

Model

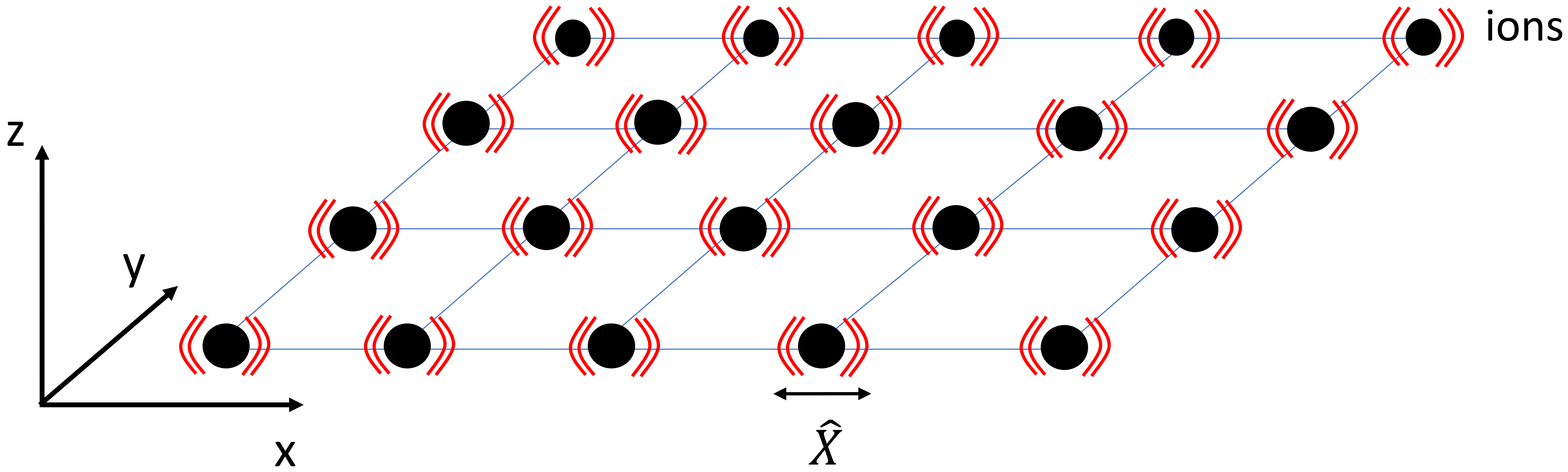
Model

Pictorial view



Model

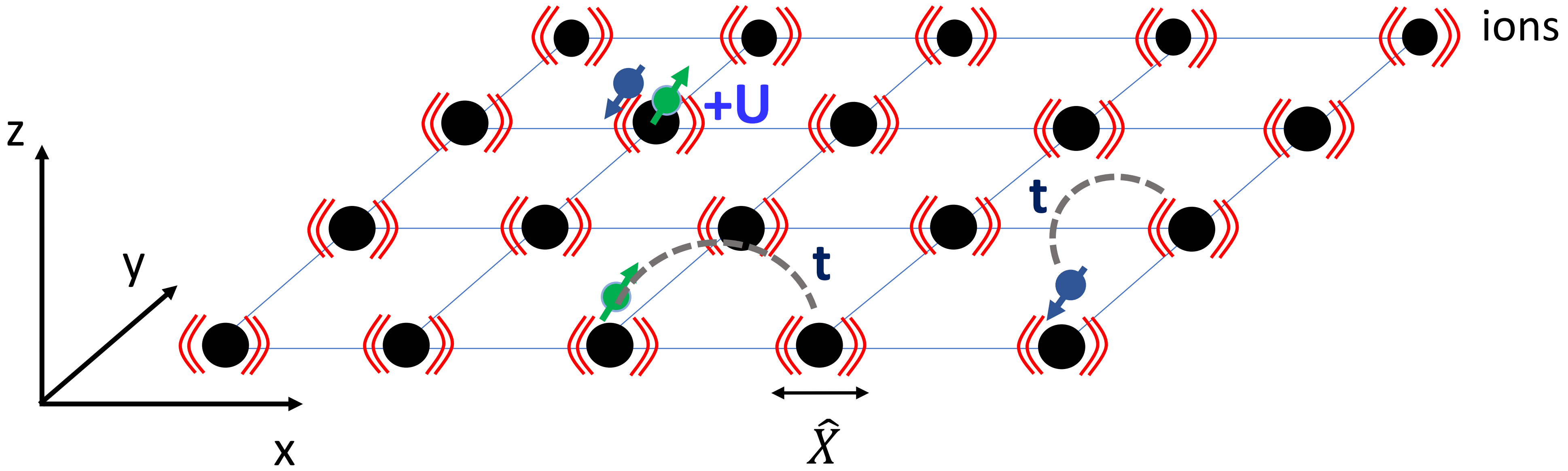
Pictorial view

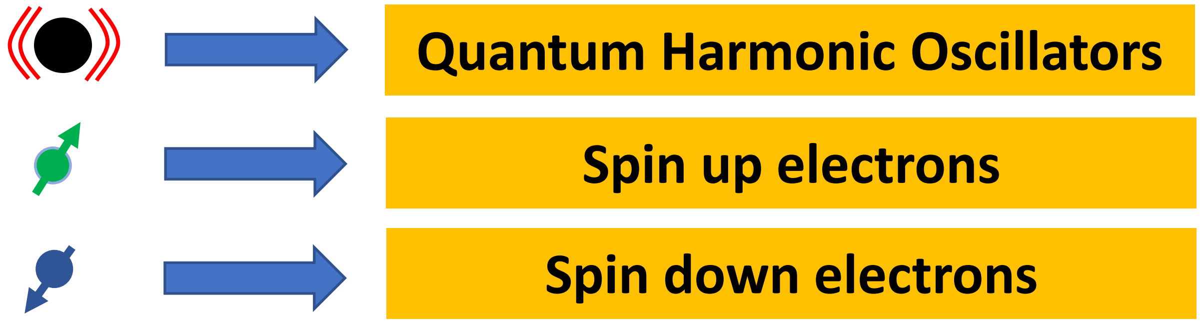


Quantum Harmonic Oscillators

Model

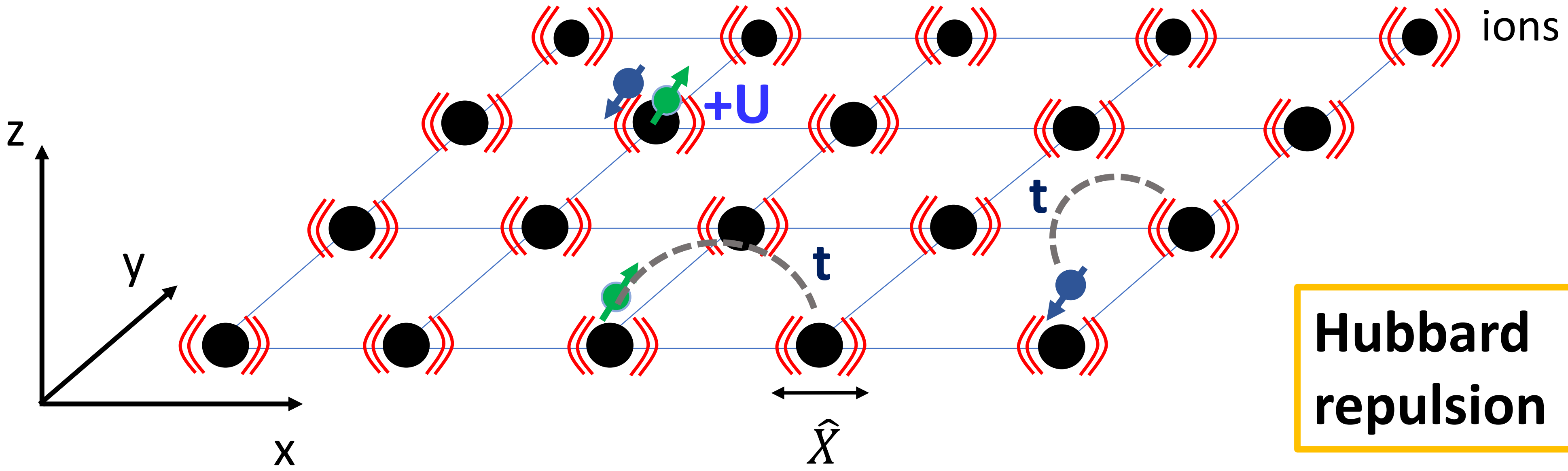
Pictorial view



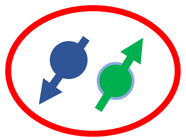


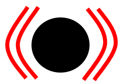
Model

Pictorial view



Hubbard repulsion

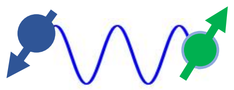


 **Quantum Harmonic Oscillators**

 **Spin up electrons**

 **Spin down electrons**

Indirect interaction mediated by phonons



Hubbard-Holstein Hamiltonian

Model

Electron hopping term

Electron-phonon interaction

$$\mathcal{H} = -t\sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma}\left(d^{\dagger}_{\mathbf{i}\sigma}d_{\mathbf{j}\sigma} + \text{h.c.}\right) - \mu\sum_{\mathbf{i},\sigma} n^{\dagger}_{\mathbf{i},\sigma} - g\sum_{\mathbf{i},\sigma} n_{\mathbf{i}\sigma}\hat{X}_{\mathbf{i}}$$

$$+ \sum_{\mathbf{i}}\left(\frac{\hat{P}^{2}_{\mathbf{i}}}{2M} + \frac{M\omega_0^2}{2}\hat{X}^{2}_{\mathbf{i}}\right) + U\sum_{\mathbf{i}} n_{\mathbf{i}\uparrow}n_{\mathbf{i}\downarrow}$$

Local Harmonic Oscillators

Hubbard interaction

Physical Quantities

Density-density Structure Factor:

$$S_{\mathrm{cdw}}(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{i},\mathbf{j}} e^{-i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\langle n_{\mathbf{i}} n_{\mathbf{j}}\rangle$$

Spin-Spin Structure Factor:

$$S_{\mathrm{afm}}(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{i},\mathbf{j}} e^{-i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\langle S^z_{\mathbf{i}} S^z_{\mathbf{j}}\rangle$$

Correlation ratio:

$$R_\nu(L) = 1 - \frac{S_\nu(\mathbf{q}+\delta\mathbf{q})}{S_\nu(\mathbf{q})}$$

$$|\delta\mathbf{q}| = 2\pi/L$$

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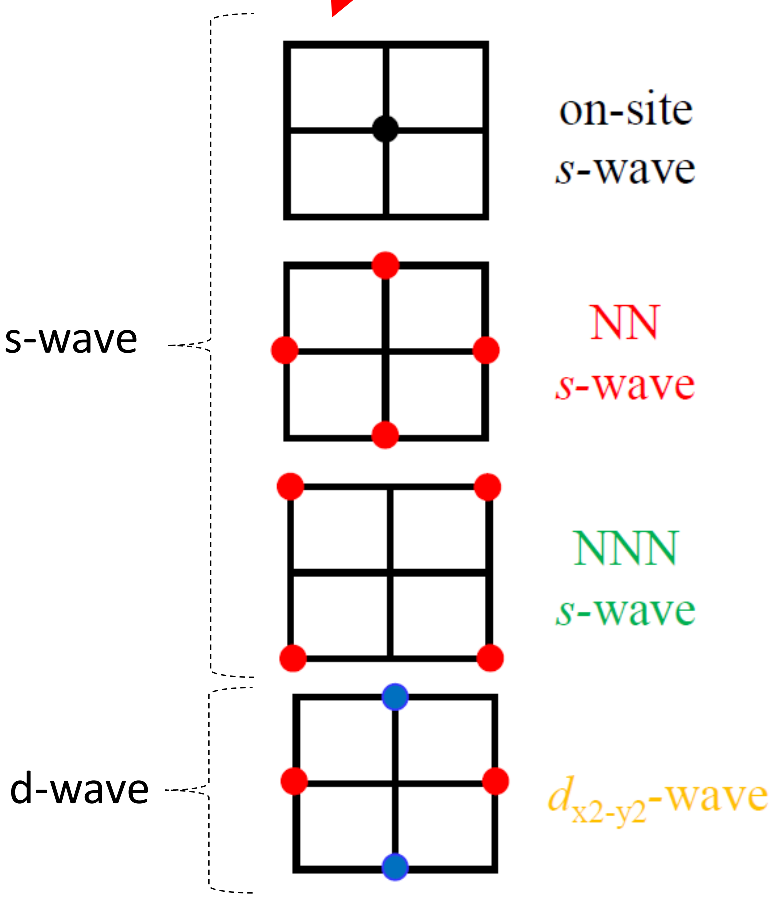
Pair Susceptibility:

$$\chi^\alpha_{\text{sc}}(\beta) = \frac{1}{N}\int_0^\beta \mathrm{d}\tau\ \langle \Delta_\alpha(\tau)\Delta^\dagger_\alpha(0)\rangle$$

$$\Delta_\alpha(\tau) = \frac{1}{2}\sum_{\mathbf{i},\mathbf{a}} f_\alpha(\mathbf{a})\, c^\dagger_{\mathbf{i}\downarrow}(\tau)\, c^\dagger_{\mathbf{i}+\mathbf{a}\uparrow}(\tau)$$



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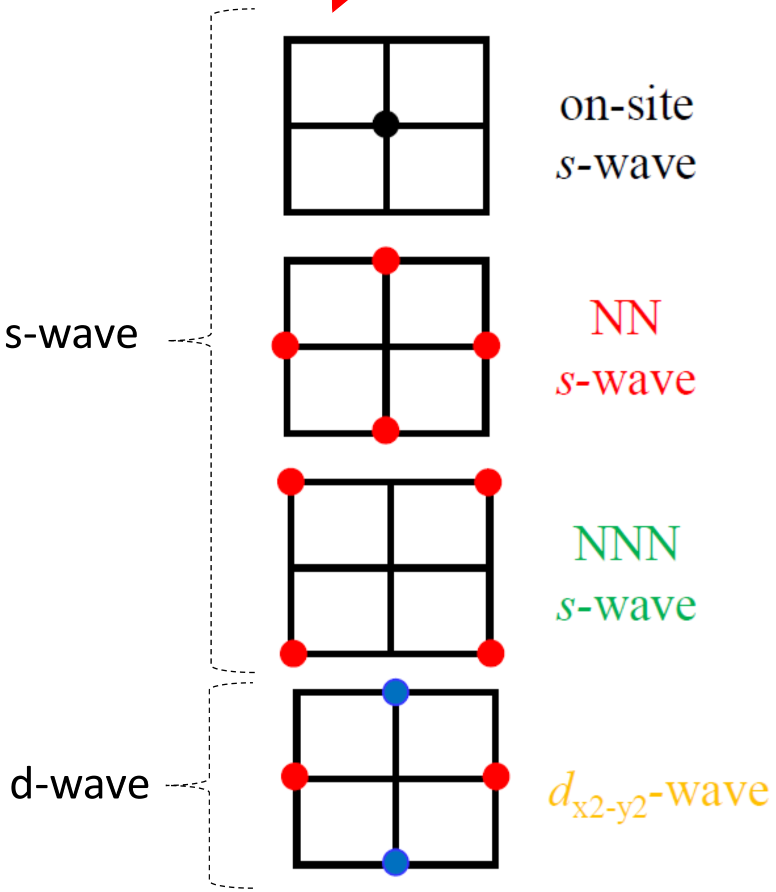


Parameters

Adiabaticity ratio:

$$\omega_0/t$$

Effective interactions:

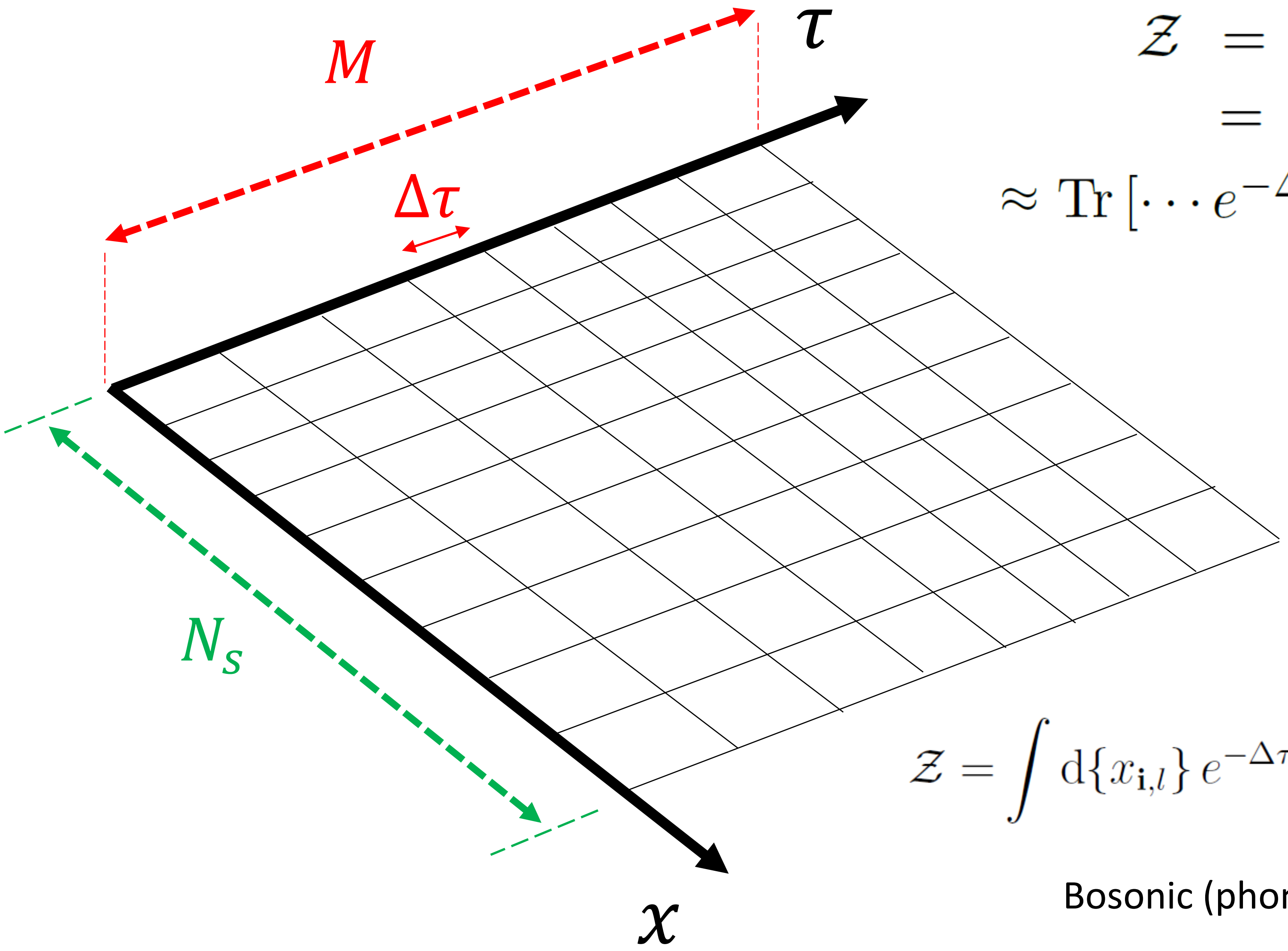
$$U_{\mathrm{eff}}(\omega) = U - \frac{g^2/\omega_0^2}{1-(\omega/\omega_0)^2}$$

$$g^2/\omega_0^2 \equiv \lambda$$

$$U_{\mathrm{eff}} \equiv U - \lambda$$

(half filling)

Method I: (finite temperature) Determinant Quantum Monte Carlo (DQMC)



$$\mathcal{Z} = \mathrm{Tr}\, e^{-\beta\hat{\mathcal{H}}}$$
$$= \mathrm{Tr}\left[\left(e^{-\Delta\tau(\hat{\mathcal{H}}_K+\hat{\mathcal{H}}_{\mathrm{U}}+\hat{\mathcal{H}}_{\mathrm{ph}}+\hat{\mathcal{H}}_{\mathrm{el-ph}})}\right)^M\right]$$
$$\approx \mathrm{Tr}\left[\cdots e^{-\Delta\tau\hat{\mathcal{H}}_K} e^{-\Delta\tau\hat{\mathcal{H}}_{\mathrm{U}}} e^{-\Delta\tau\hat{\mathcal{H}}_{ph}} e^{-\Delta\tau\hat{\mathcal{H}}_{\mathrm{el-ph}}}\cdots\right]$$

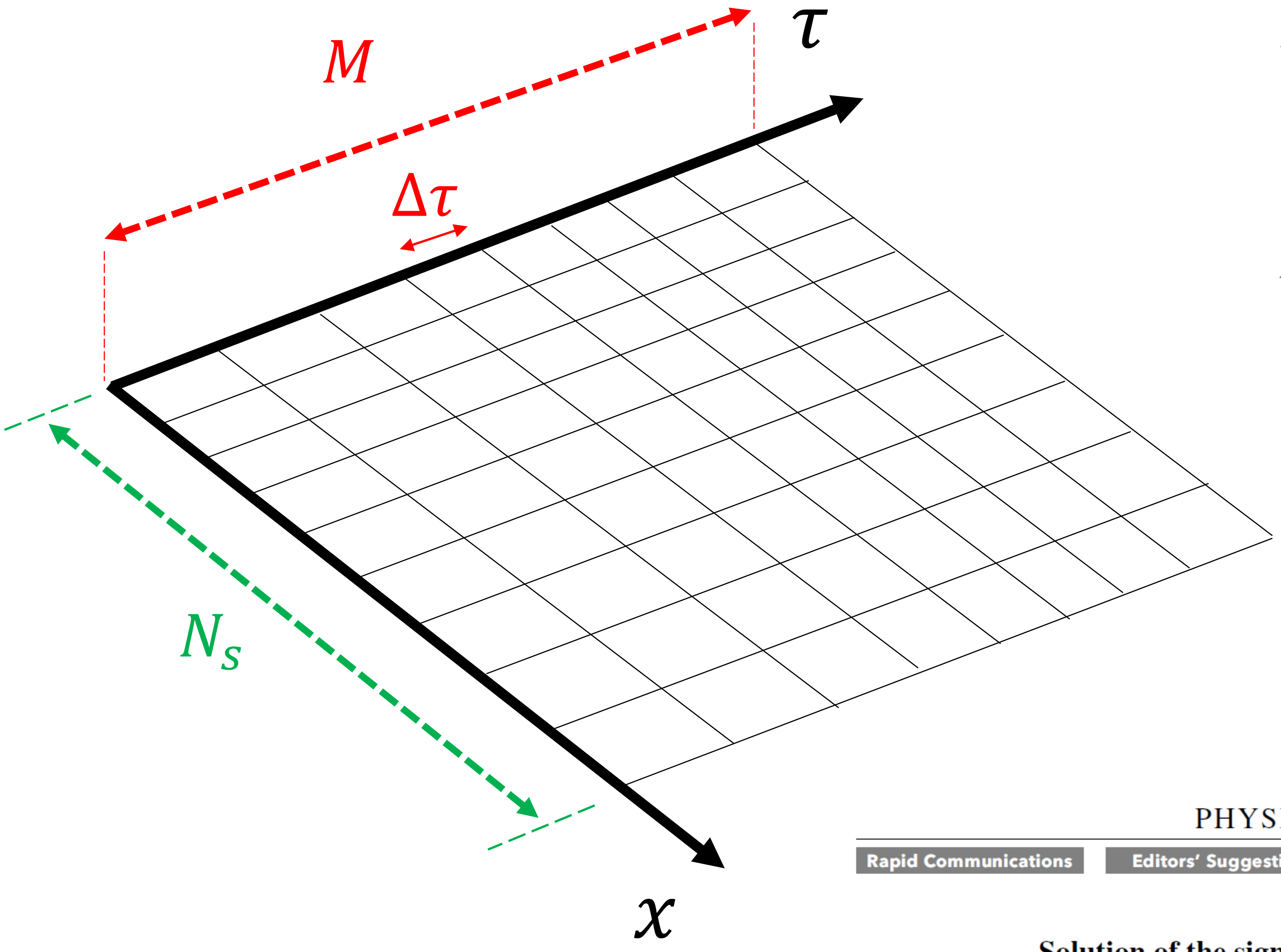
$$\mathcal{Z} = \int \mathrm{d}\{x_{\mathrm{i},l}\}\, e^{-\Delta\tau S_B} \prod_\sigma \left[\det\left[I + B^\sigma(M)B^\sigma(M-1)\cdots B^\sigma(1)\right]\right]$$

Bosonic (phonon) action: $S_B = \sum_{\mathrm{i}}\sum_{l=1}^{M}\left[\frac{1}{2}\left(\frac{x_{\mathrm{i},l}-x_{\mathrm{i},l+1}}{\Delta\tau}\right)^2 + \frac{\omega_0^2}{2}x_{\mathrm{i},l}^2\right]$

$$B_l^{\uparrow(\downarrow)} = e^{\mp\Delta\tau\alpha v(l) - \Delta\tau g X(l)} e^{-\Delta\tau K}$$

⇨ Minus-sign problem even at the half-filling!! (It depends on the system size, temperature, and interaction strength)

Method II: (projective) Auxiliary-field Quantum Monte Carlo (AFQMC)



$$\mathcal{Z} = \lim_{\beta\to\infty} \langle \psi_L | e^{-\beta\mathcal{H}} | \psi_R \rangle$$

$$\mathcal{Z} = \lim_{\beta\to\infty} \prod_{\sigma} \langle 0 | \left(\Phi_L^{\sigma} \mathbf{c}_{\sigma} \right) e^{-\beta\mathcal{H}} \left(\mathbf{c}_{\sigma}^{\dagger} \Phi_R^{\sigma} \right) | 0 \rangle$$

$$\mathcal{Z} = \prod_{\sigma} \det \left[\Phi_L^{\sigma} \mathbf{B}(2\tau_F, 0) \Phi_R^{\sigma} \right]$$

- Inversion sampling algorithm for singles moves (~~accept-reject~~)
- Integrate out the phonon fields
  - No autocorrelation problem!
  - It is sign-free for $U_{eff} \geq 0$

Severe sign problem for $U_{eff} < 0$

PHYSICAL REVIEW B **98**, 201108(R) (2018)

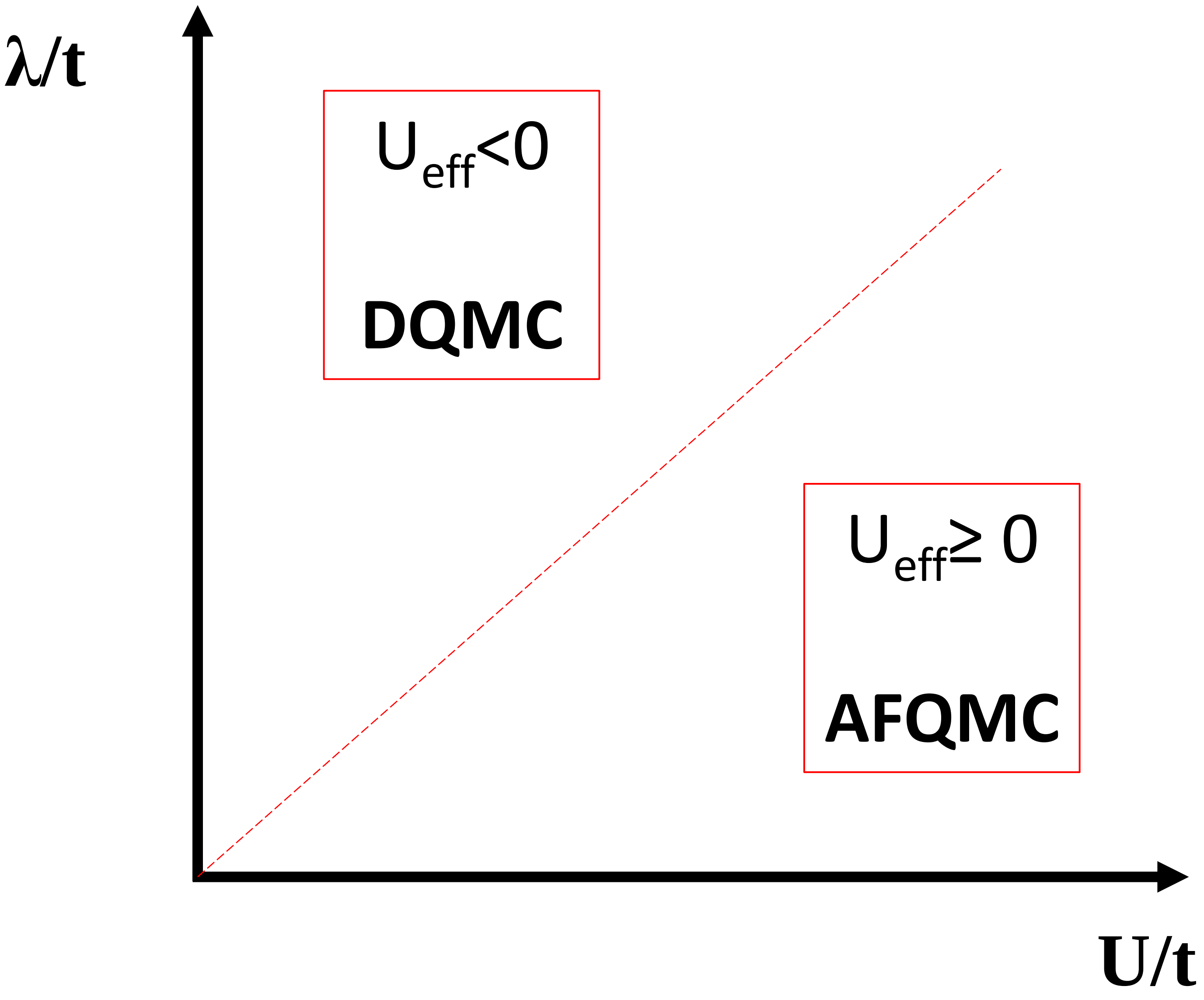
Rapid Communications | Editors' Suggestion

Solution of the sign problem for the half-filled Hubbard-Holstein model

Seher Karakuzu,[1] Kazuhiro Seki,[1,2,3] and Sandro Sorella[1,2]

[1]*International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy*
[2]*Computational Materials Science Research Team, RIKEN Center for Computational Science (R-CCS), Hyogo 650-0047, Japan*
[3]*Computational Condensed Matter Physics Laboratory, RIKEN Cluster for Pioneering Research (CPR), Saitama 351-0198, Japan*

Here, we fixed $\beta \sim L^z$, with L being the linear size of the lattice, and $z=1$ and 2.



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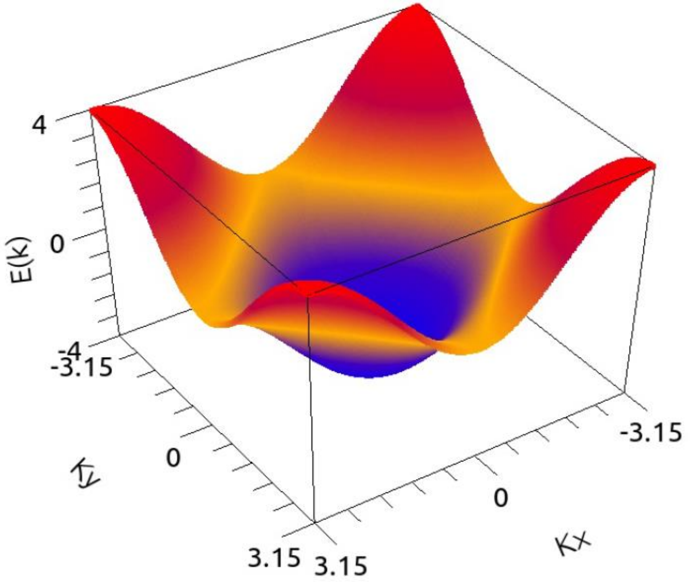
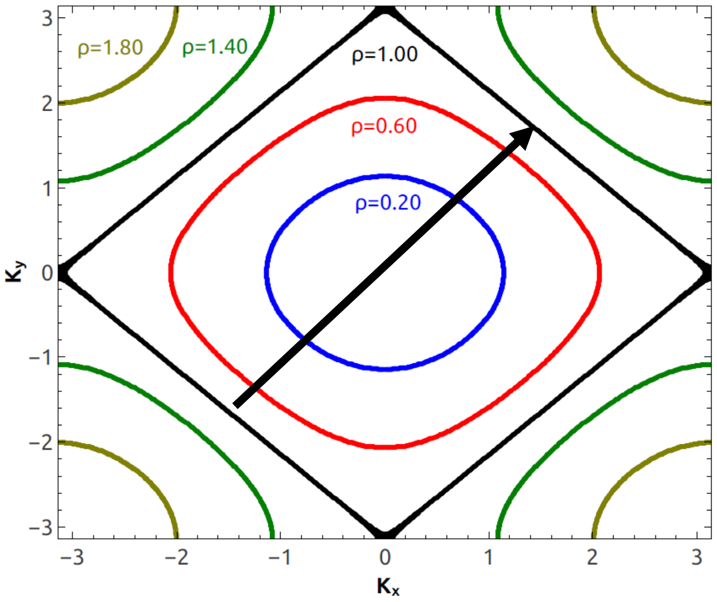
Important …

Square lattice exhibits FSN and van Hove singularity at half filling



CDW and AFM Instabilities

Fermi Surface



The pure Holstein model (U=0)

In absence of Hubbard interaction (i.e., for the pure Holstein model) CDW is expected for any EPI.

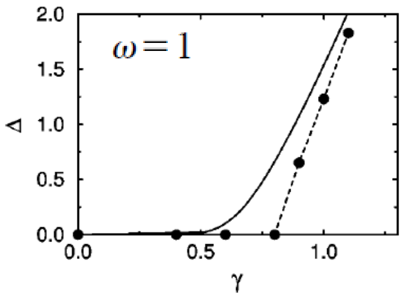
HOWEVER, in 1D a finite EPC is required for CDW

PHYSICAL REVIEW B VOLUME 60, NUMBER 11 15 SEPTEMBER 1999-I

Metal-insulator transition in the one-dimensional Holstein model at half filling

Eric Jeckelmann,* Chunli Zhang, and Steven R. White
Department of Physics and Astronomy, University of California, Irvine, California 92697
(Received 10 March 1999)

DMRG



Metal-insulator transition from a Luther-Emery liquid to a charge ordered phase.

Review paper…

Eur. Phys. J. B (2018) 91: 204
https://doi.org/10.1140/epjb/e2018-90354-7
THE EUROPEAN PHYSICAL JOURNAL B

Colloquium

Density waves in strongly correlated quantum chains*

Martin Hohenadler[1,a] and Holger Fehske[2,b]

[1] Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany
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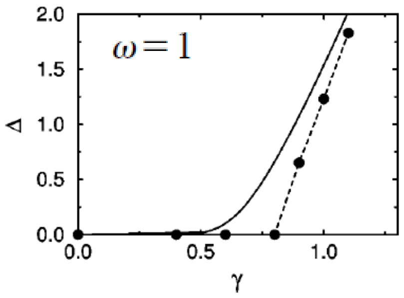

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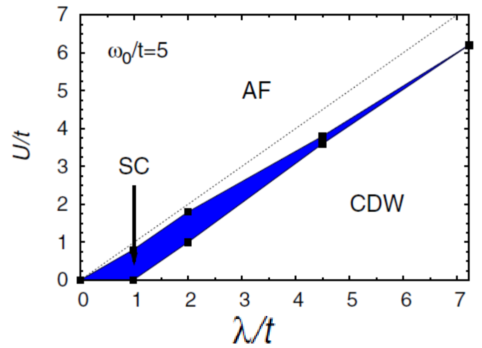
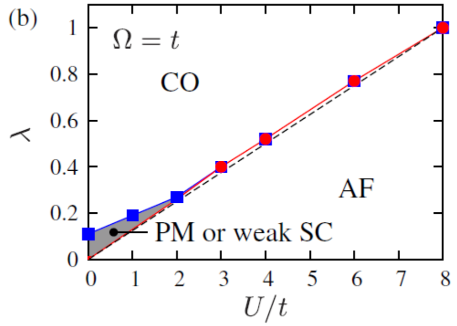
How about the square lattice?

Variational Monte Carlo approaches



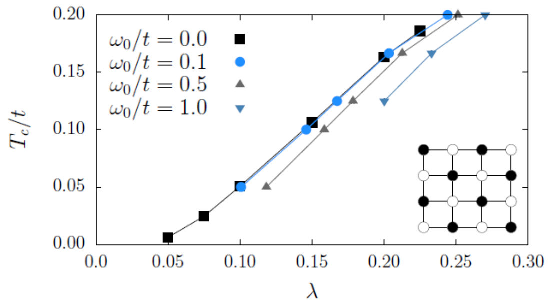
S. Karakuzu, et.al, PRB **98**, 201108 (2018)



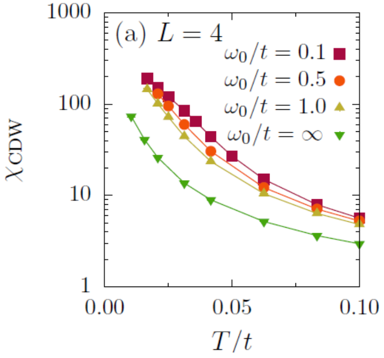
T. Ohgoe, et. al, PRL **119**, 197001 (2017)

QCP for a finite EPC!

Quantum Monte Carlo approaches



M. Weber, et. al, PRB **98**, 085405 (2018)



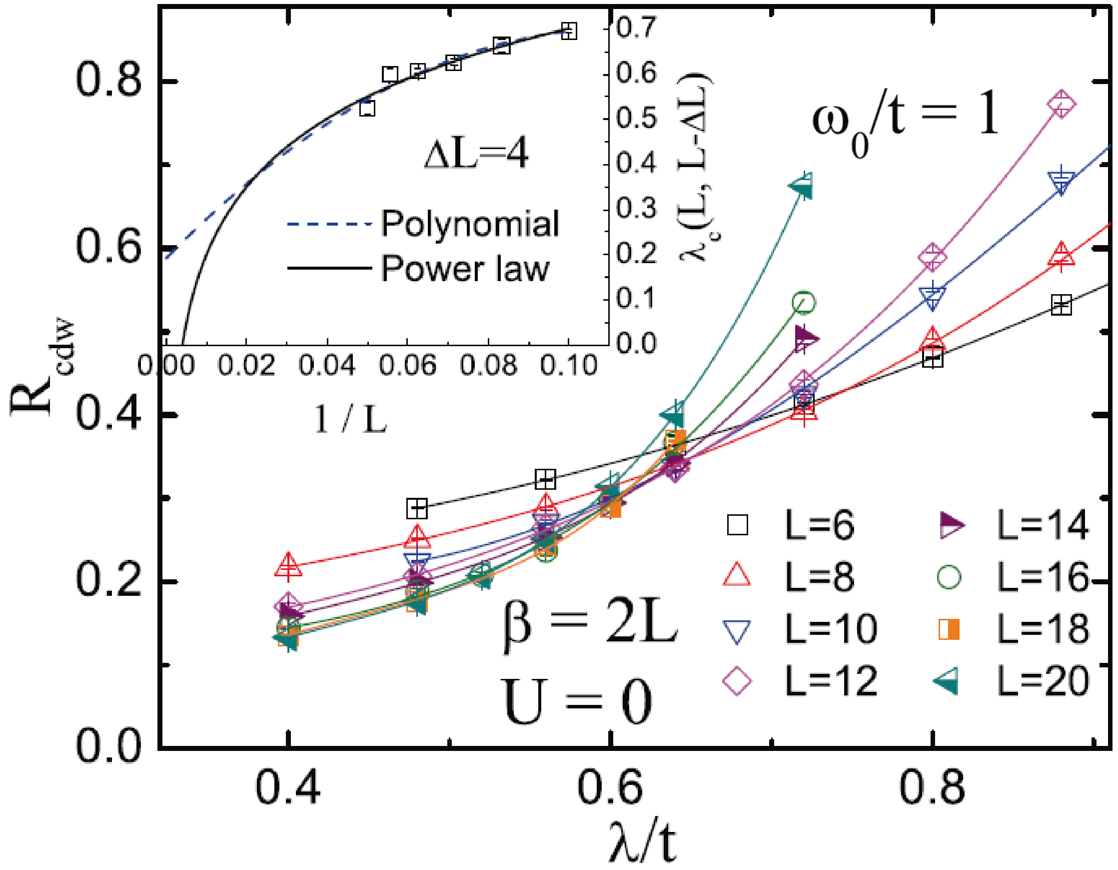
M. Hohenadler et. al, PRB **100**, 165114 (2019)

CDW for any EPC!

The pure Holstein model (U=0)

DQMC Method

$$R_\nu(L) = 1 - \frac{S_\nu(\mathbf{q}+\delta\mathbf{q})}{S_\nu(\mathbf{q})}$$



$$f(L) = a + bL^c$$

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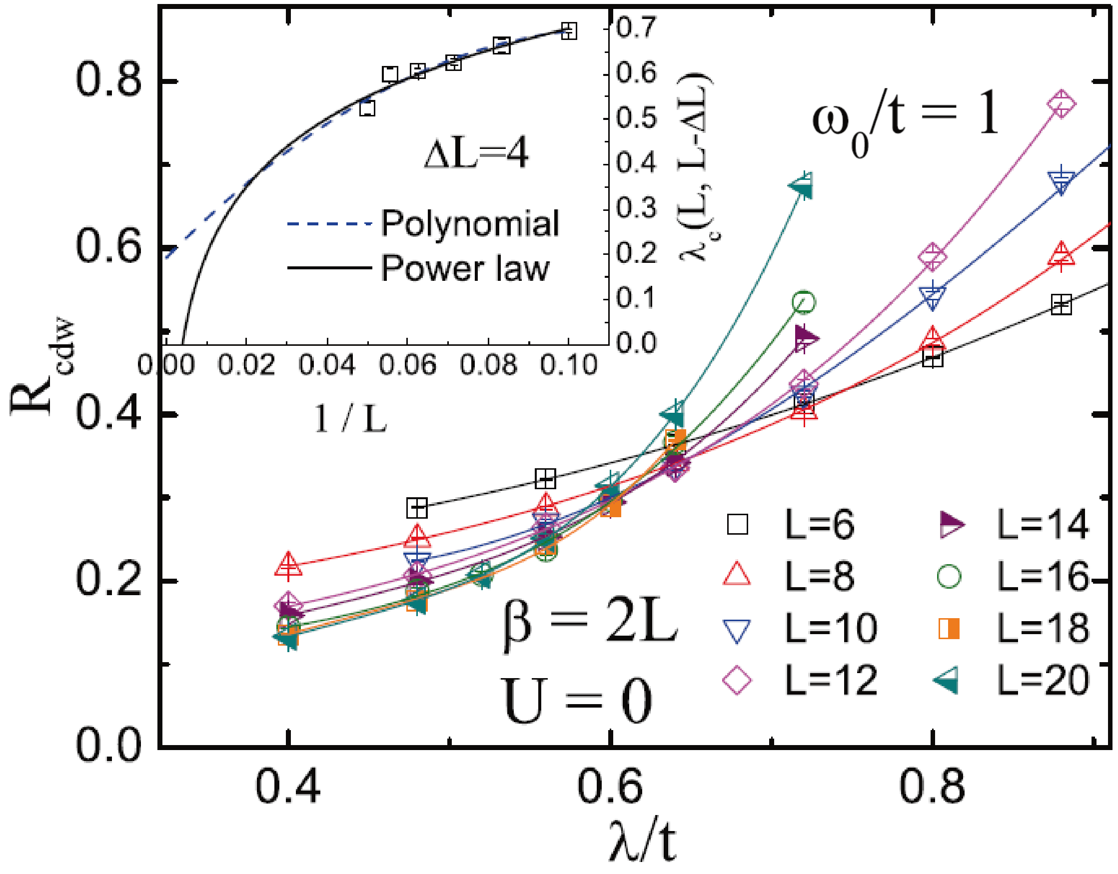

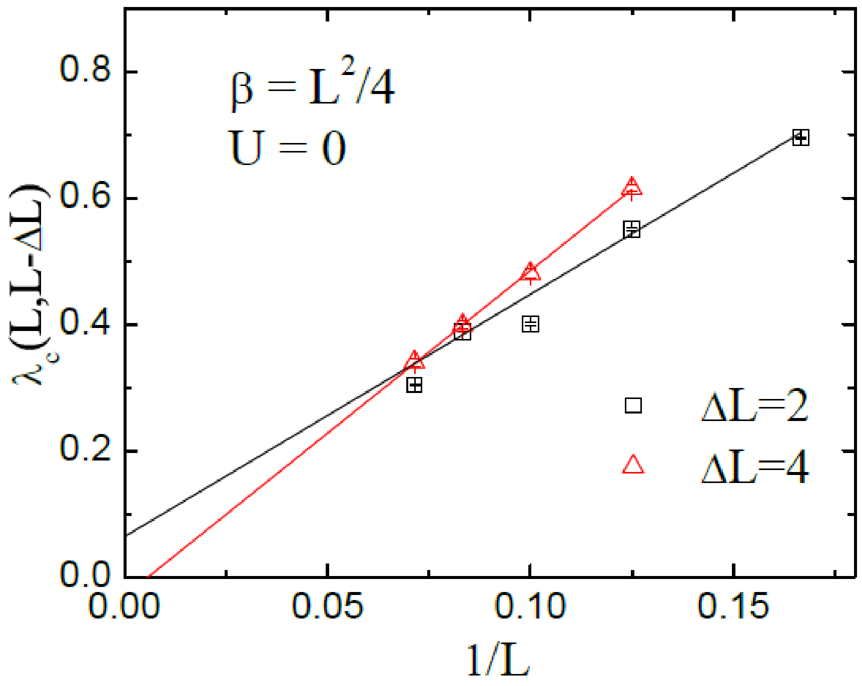

No finite critical electron-phonon coupling for CDW for the pure Holstein model!!

$$f(L) = a + bL^c$$

The Hubbard-Holstein model (U=λ)

AFQMC Method

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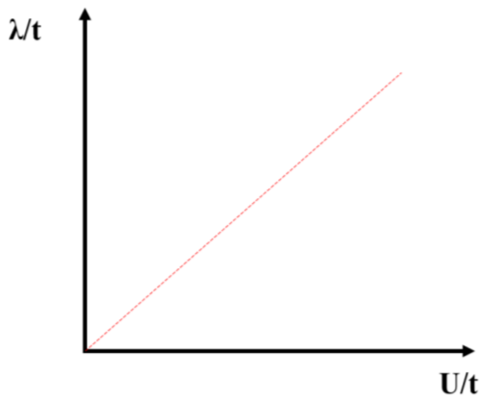

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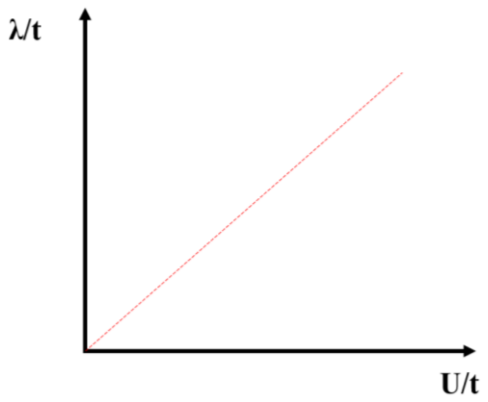

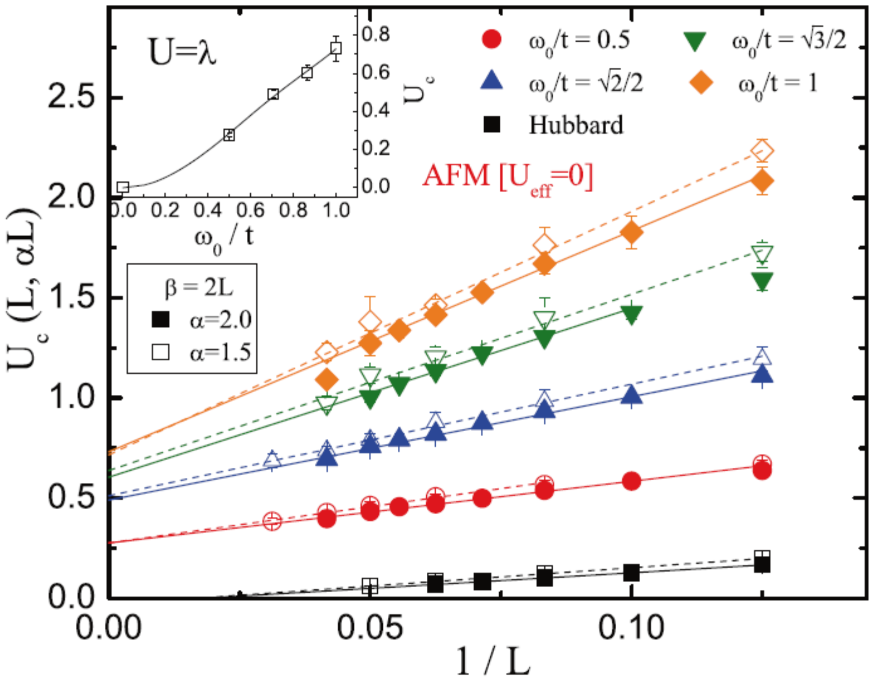

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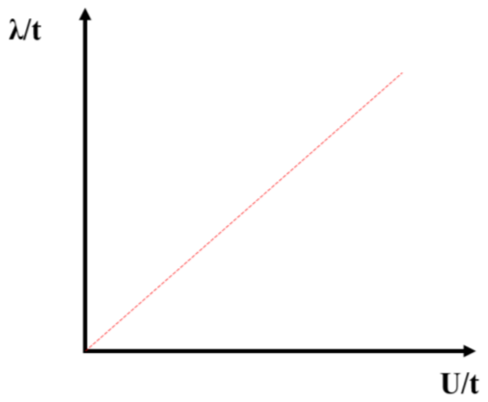
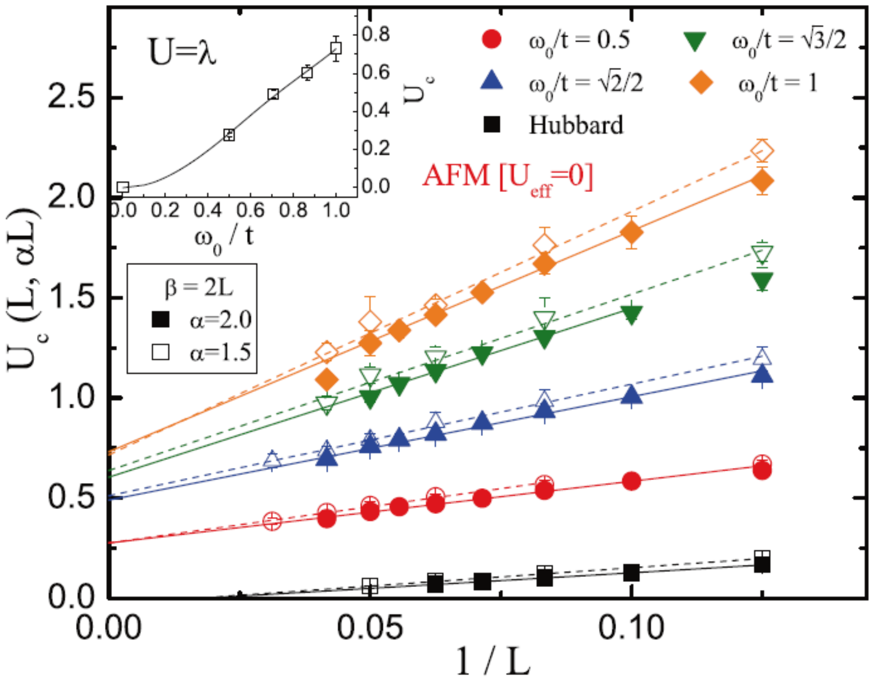
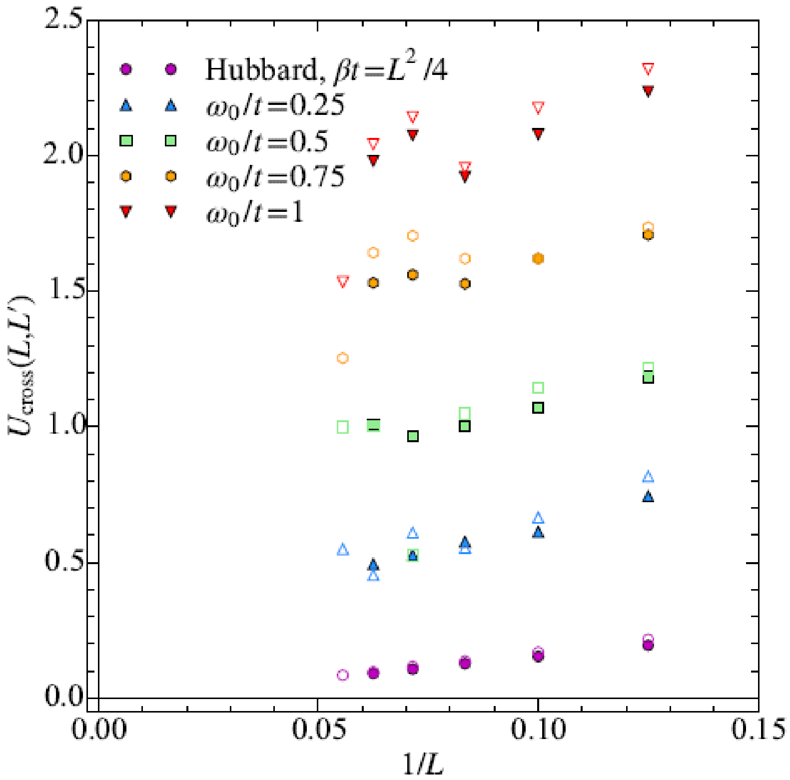






AFM QCP for U=λ !
Spin fluctuations are stronger than charge ones.

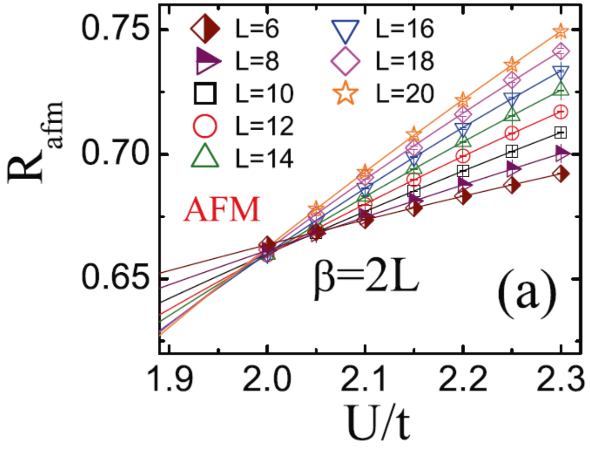
Metal-Insulator transition?

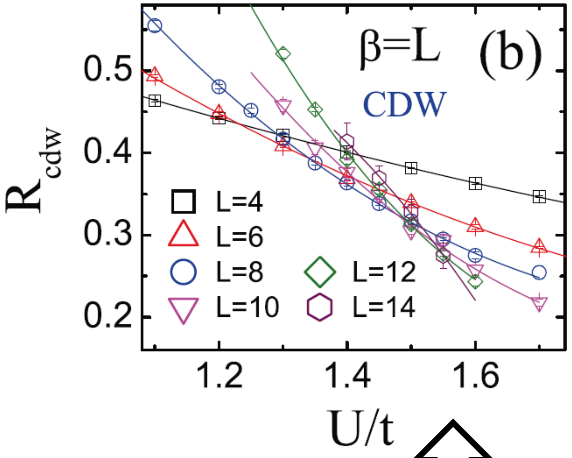
The Hubbard-Holstein model (U≠λ)

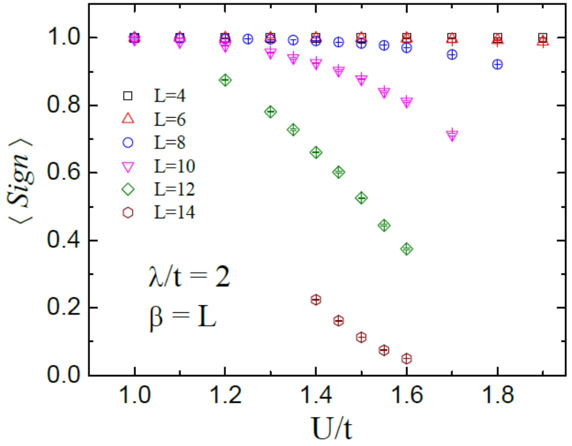
AFQMC and DQMC Methods

$\lambda/t=2 \qquad \omega_0/t = 1$

$$R_\nu(L) = 1 - \frac{S_\nu(\mathbf{q}+\delta\mathbf{q})}{S_\nu(\mathbf{q})}$$







(DQMC) Average fermionic sign

The Hubbard-Holstein model (U≠λ)

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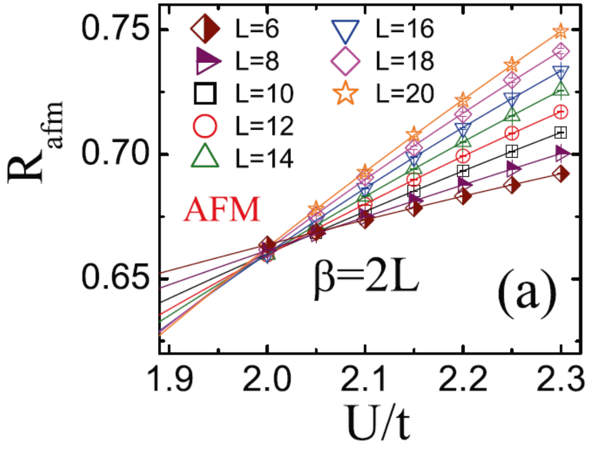
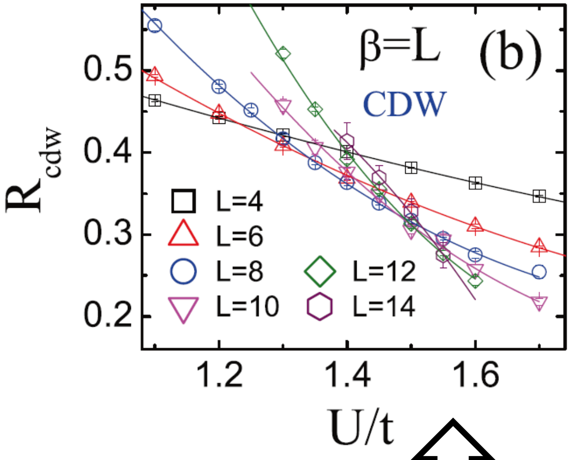
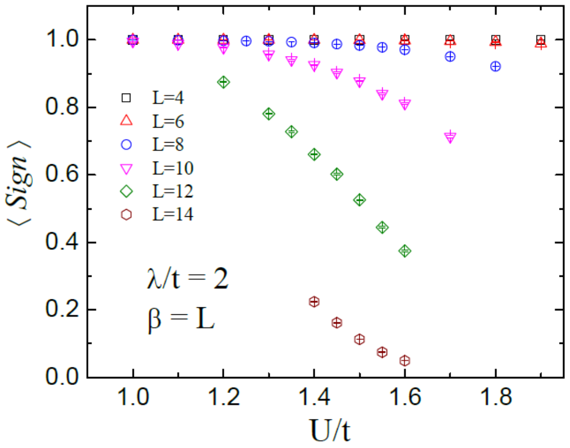
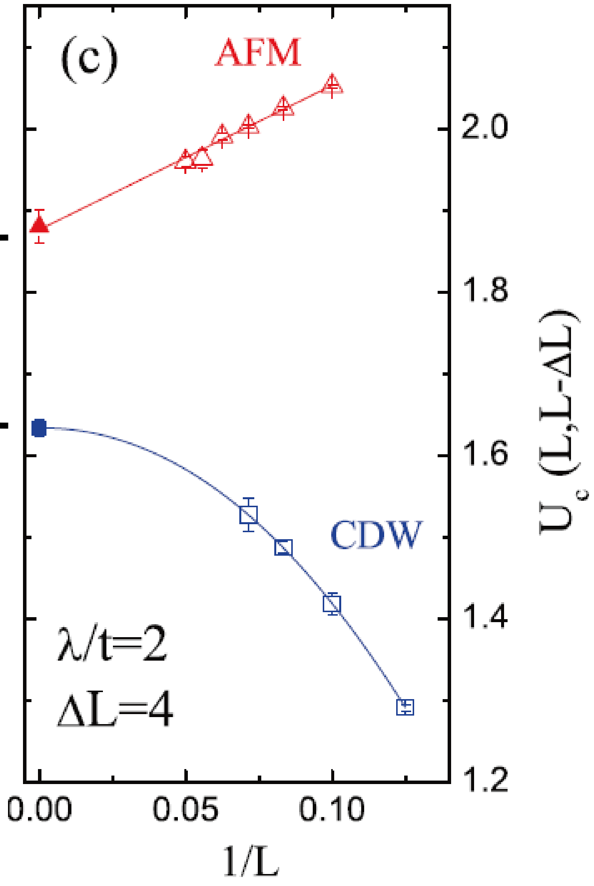




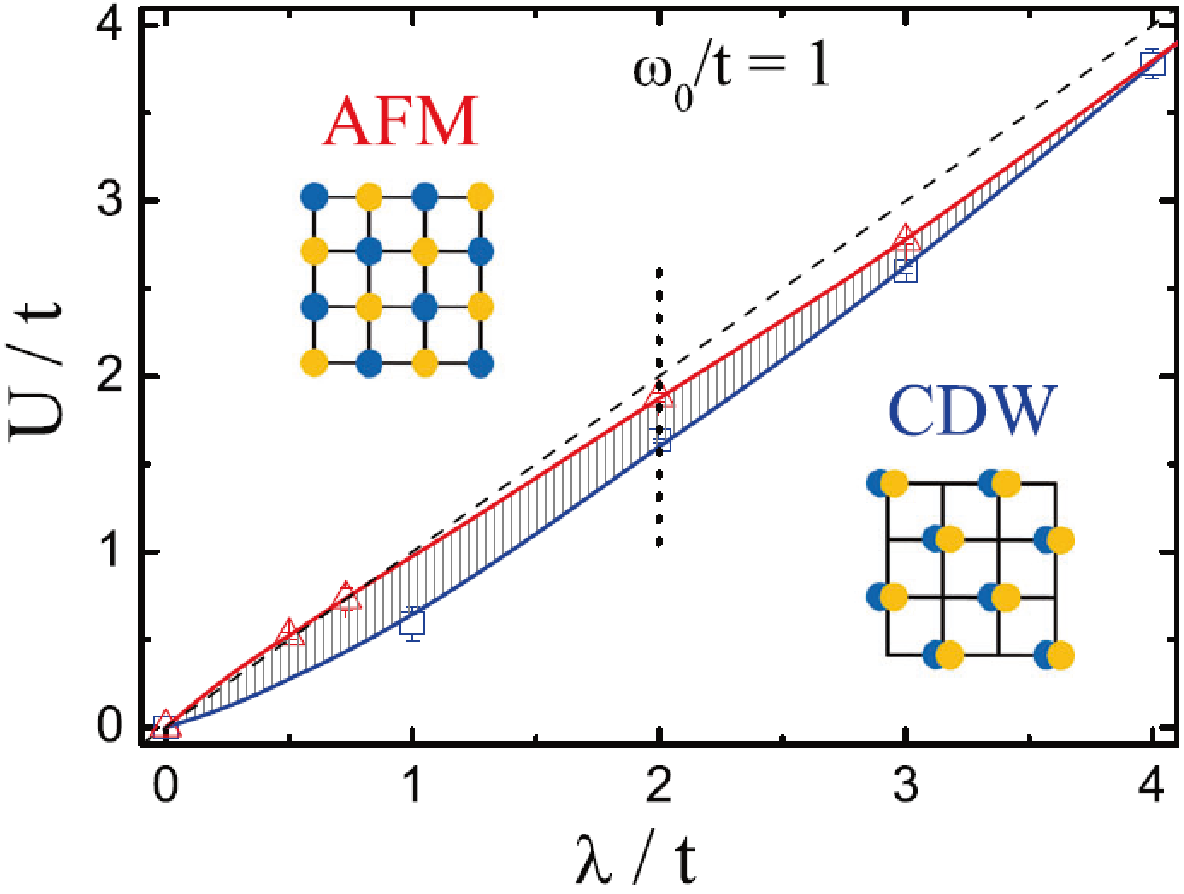


(DQMC) Average fermionic sign



No CDW, no AFM.
Metal or superconductor ?

The phase diagram of the Hubbard-Holstein model



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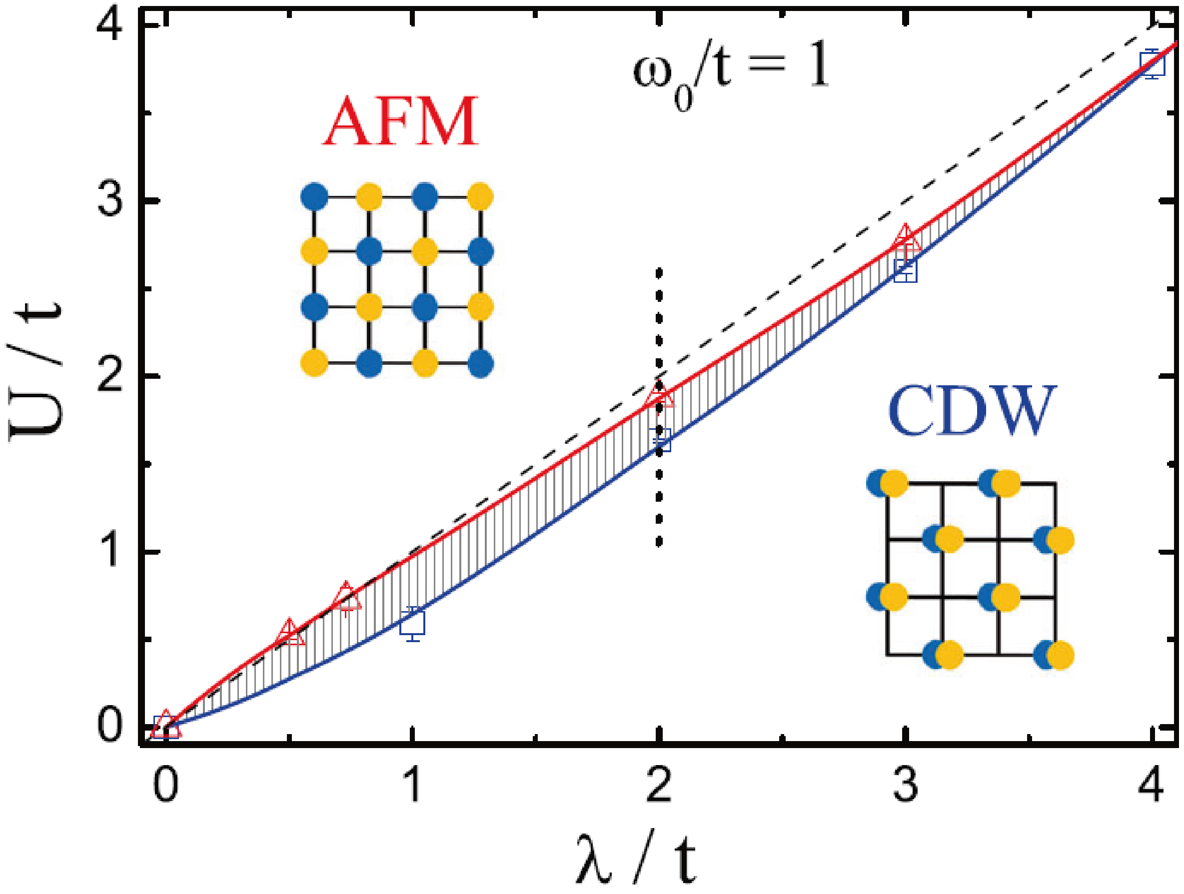


Metal or superconductor ?

$$\chi^{\text{eff}}_{\alpha(\text{sc})} = \chi_{\alpha(\text{sc})} - \bar{\chi}_{\alpha(\text{sc})}$$

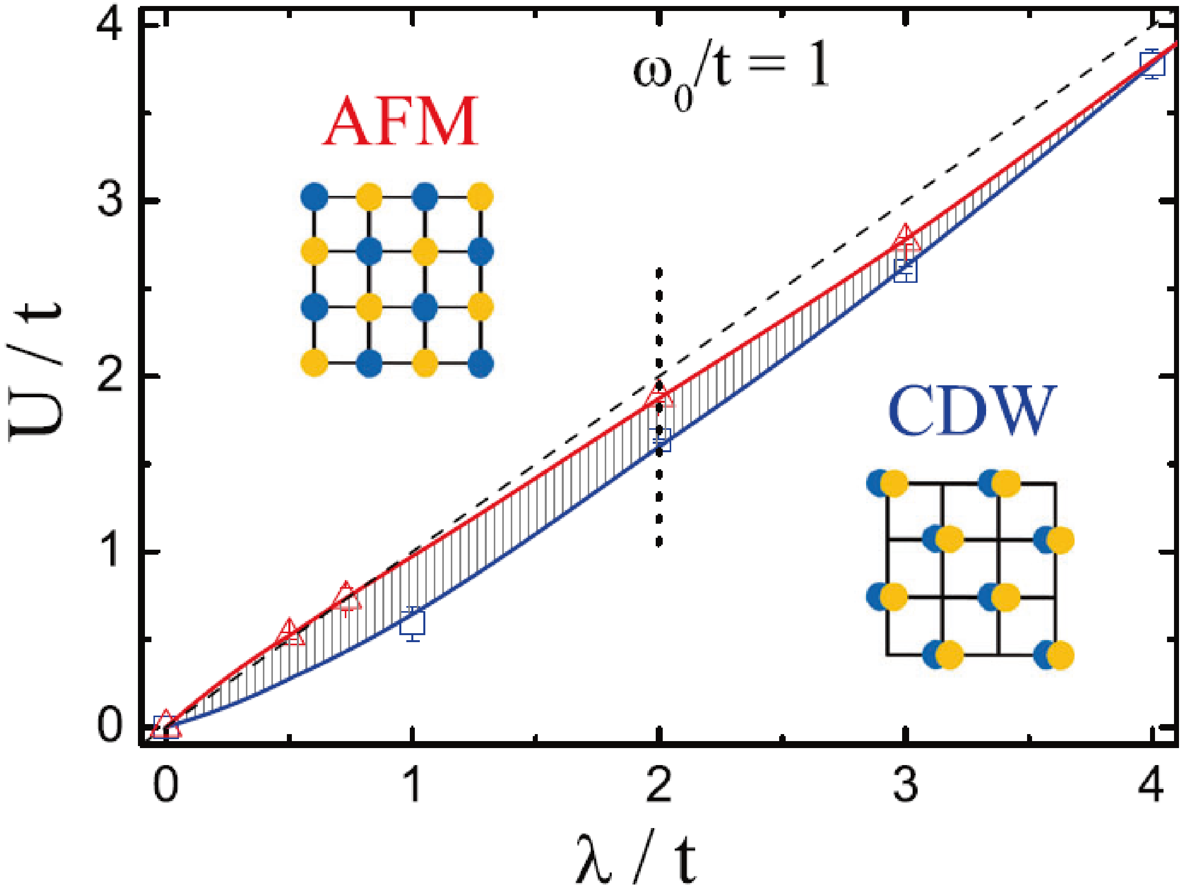
> 0 att. channel

< 0 ~~att. channel~~

decoupled contributions

$$\langle c^{\dagger}_{\mathbf{i}\downarrow}(\tau)\, c_{\mathbf{j}\downarrow}(0)\rangle \langle c^{\dagger}_{\mathbf{k}\uparrow}(\tau)\, c_{\mathbf{l}\uparrow}(0)\rangle$$

The phase diagram of the Hubbard-Holstein model



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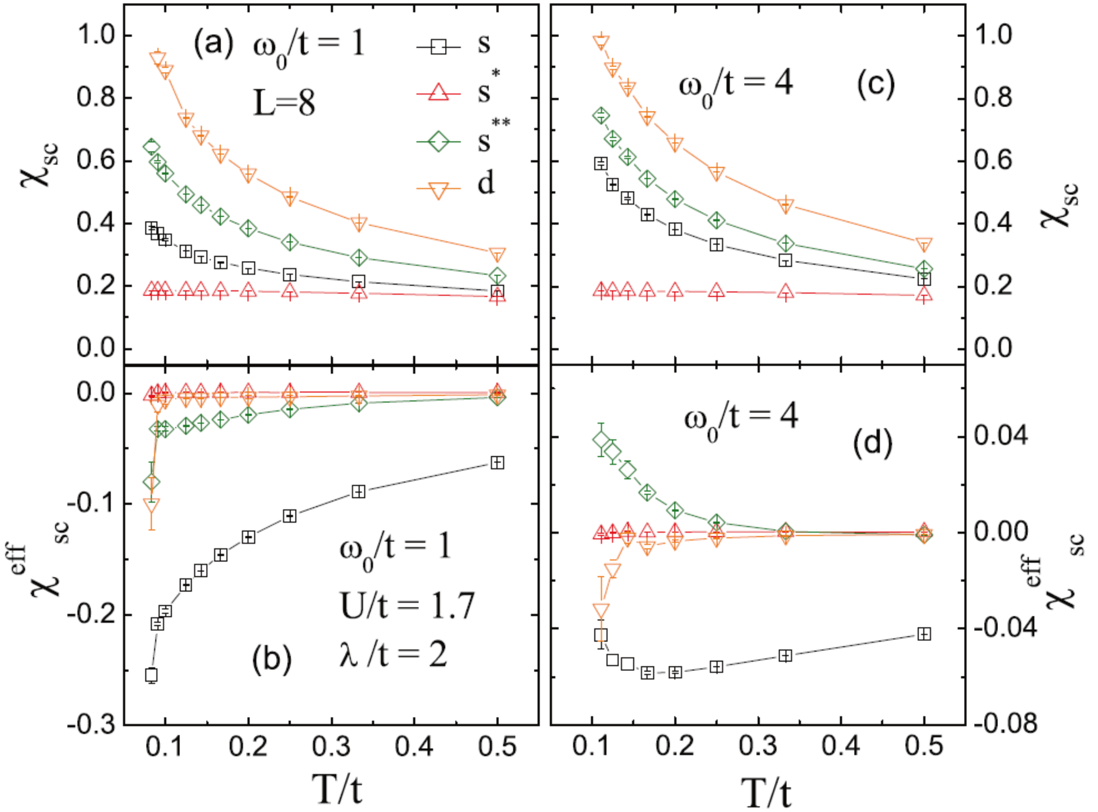

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$$\langle c^\dagger_{\mathbf{i}\downarrow}(\tau)\, c_{\mathbf{j}\downarrow}(0)\rangle \langle c^\dagger_{\mathbf{k}\uparrow}(\tau)\, c_{\mathbf{l}\uparrow}(0)\rangle$$

s-wave

Partial Conclusions

- No finite critical electron-phonon coupling for CDW in the pure Holstein model;
- Existence of a metal-AFM transition on the line $U=\lambda$, with its critical coupling strength depending on ω_0;
- First unbiased phase diagram for the HHM in the square lattice;
- Existence of a metallic-like region between CDW and AFM, with an enhancement of nonlocal s-wave pairing.

COMMUNICATIONS PHYSICS

ARTICLE

https://doi.org/10.1038/s42005-020-0342-2 OPEN

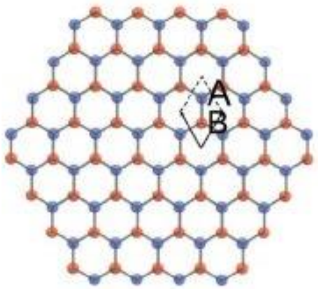
Phase diagram of the two-dimensional Hubbard-Holstein model

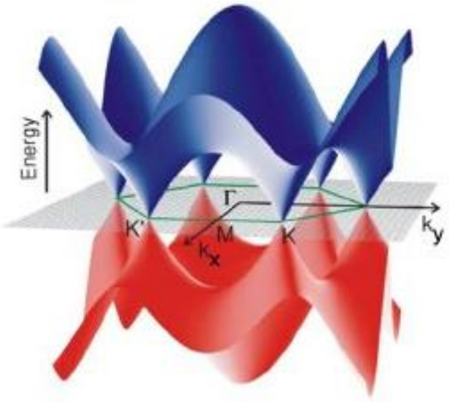
Natanael C. Costa[1,2], Kazuhiro Seki[3], Seiji Yunoki[3,4,5] & Sandro Sorella[1]

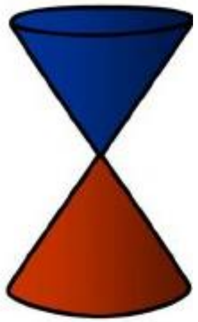
Outline

- Introduction
  - Peierls Instability and CDW formation
  - Experimental motivation
- The model and methodology
- Results
  - CDW, AFM and paring in the square lattice
  - CDW and AFM in the honeycomb lattice
- Outlooks

Honeycomb lattice



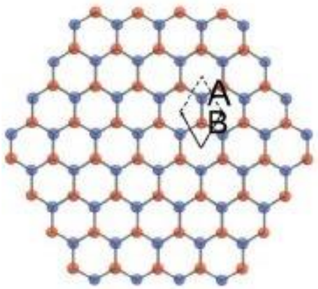


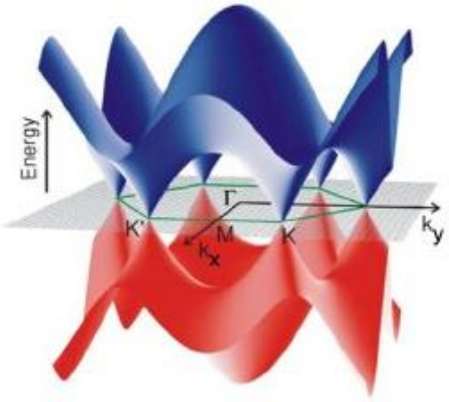


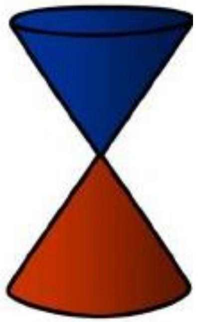
Vanishing Density of States (half-filling)

- Finite U for AFM;
- Finite λ for CDW;
- Suppression of pairing

Honeycomb lattice







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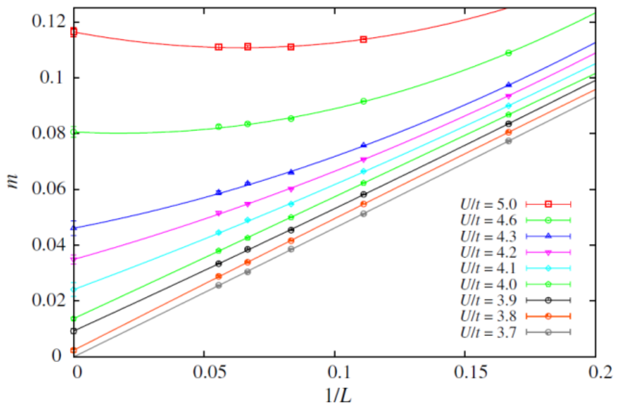
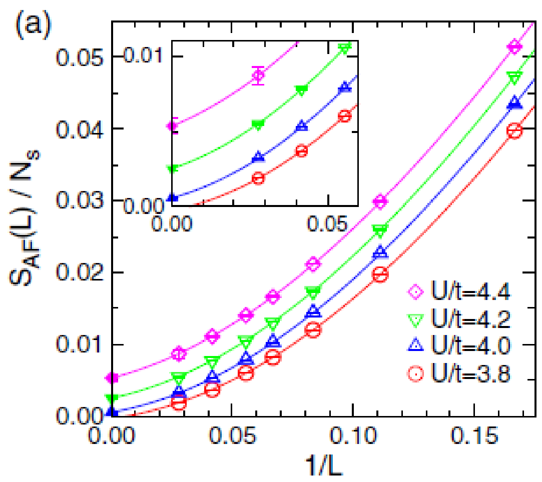
Pure Hubbard model

$U_c \approx 3.8\ t$



F. Assaad et.al, PRX **3**, 031010 (2013)



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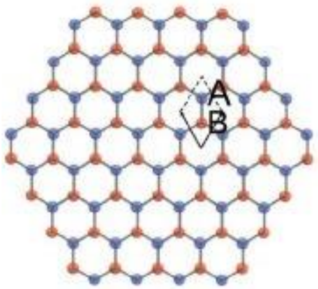
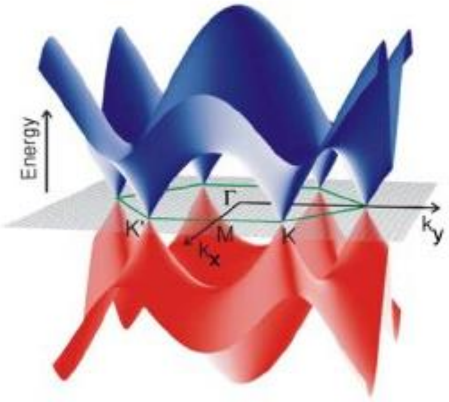
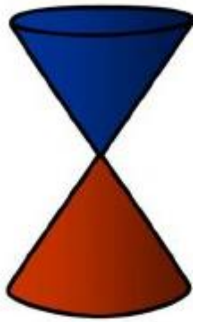
Honeycomb lattice







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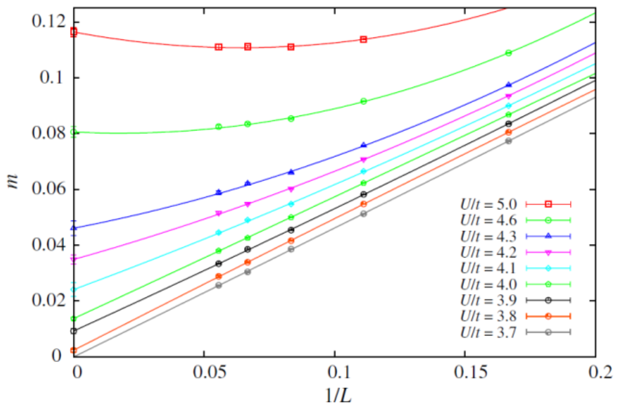

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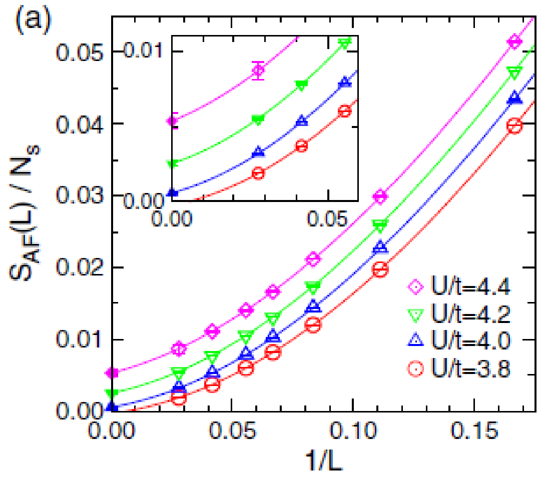
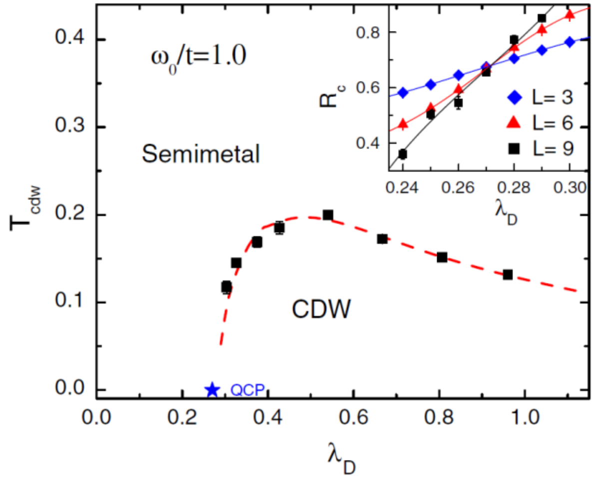


Y. Otsuka et.al, PRX **6**, 011029 (2016)

Pure Holstein model

$\lambda_c \approx 1.60t \ (\omega/t=1)$



Y-X Zhang et.al, PRL **122**, 077602 (2019)

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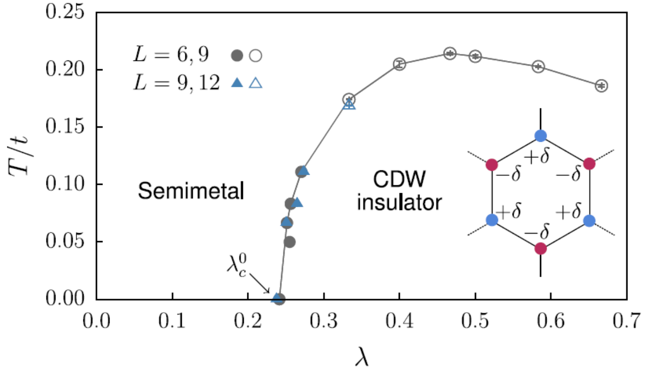
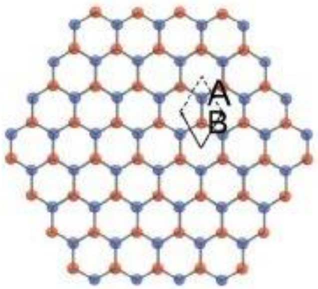
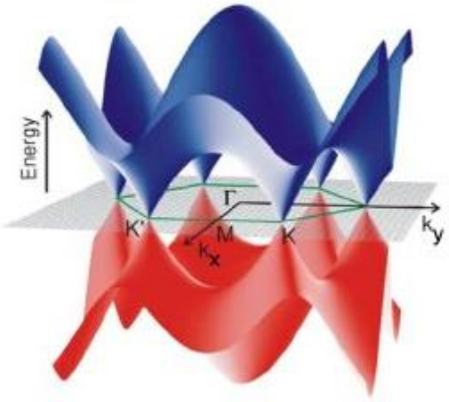
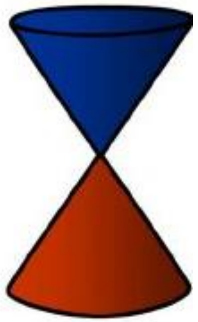


C. Chen, *et.al*, Phys. Rev. Lett. **122**, 077601 (2019)

Honeycomb lattice







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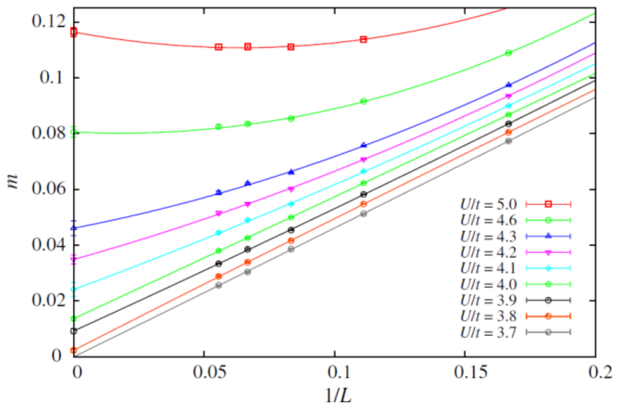

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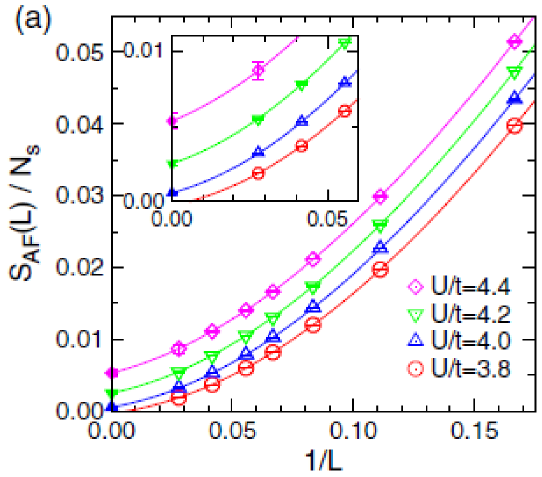

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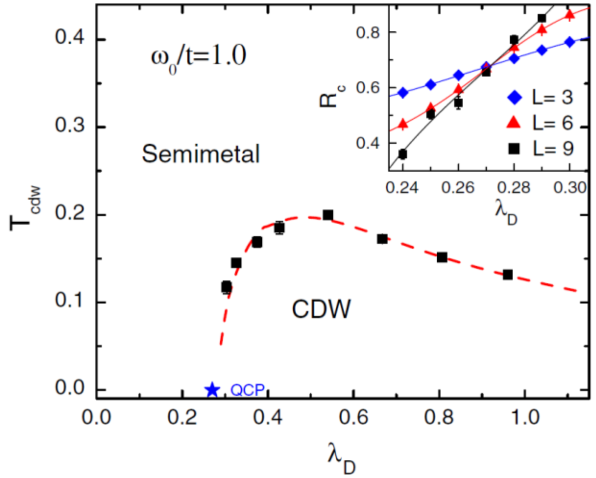

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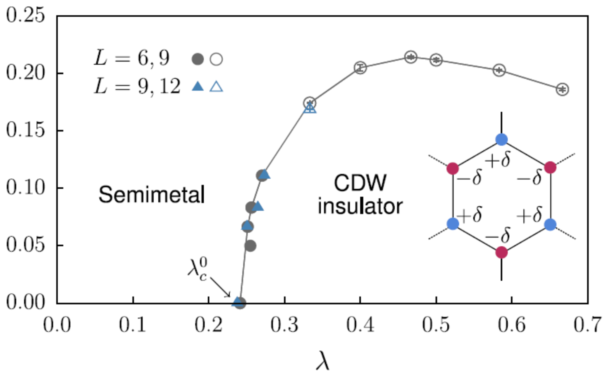
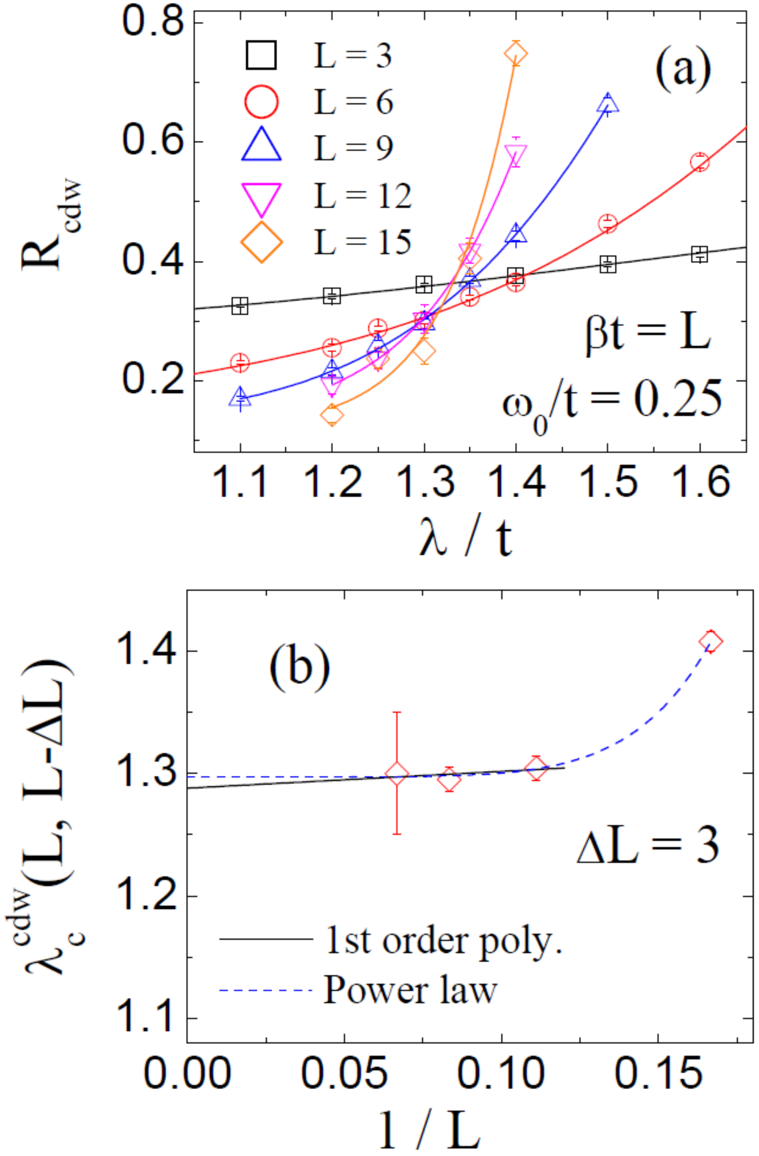


C. Chen, *et.al*, Phys. Rev. Lett. **122**, 077601 (2019)

The pure Holstein model (U=0)

DQMC Method $$R_\nu(L) = 1 - \frac{S_\nu(\mathbf{q}+\delta\mathbf{q})}{S_\nu(\mathbf{q})}$$



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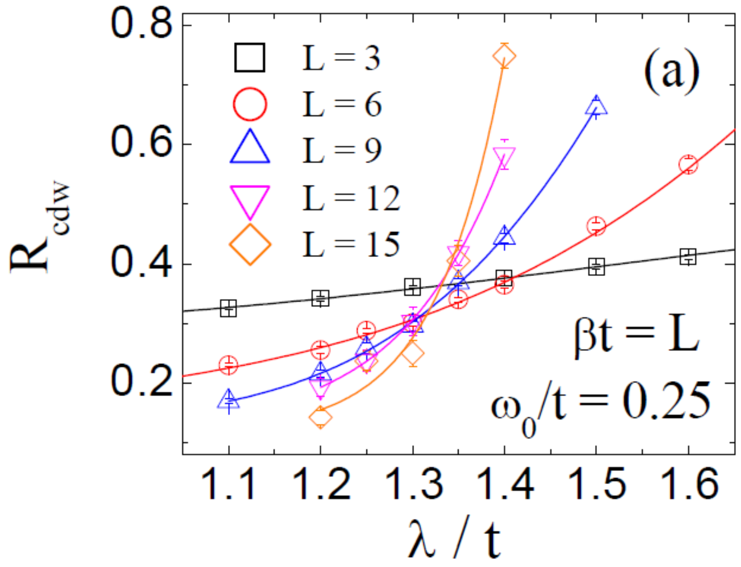

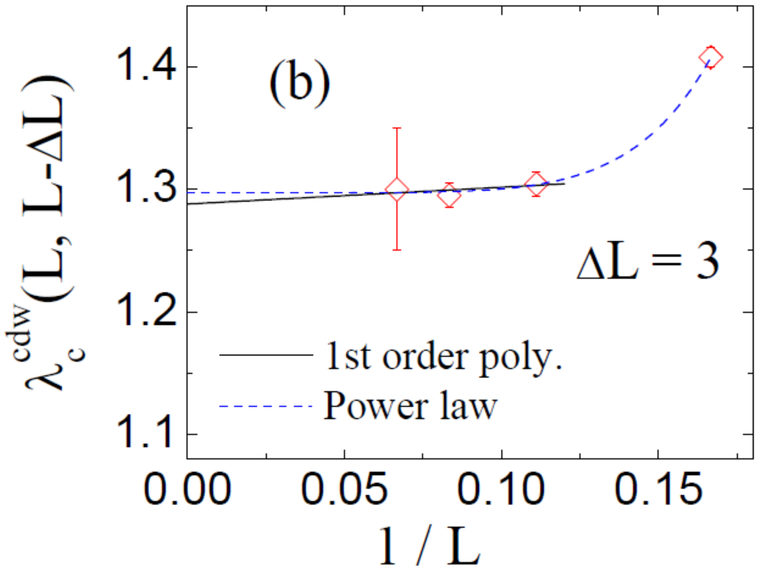

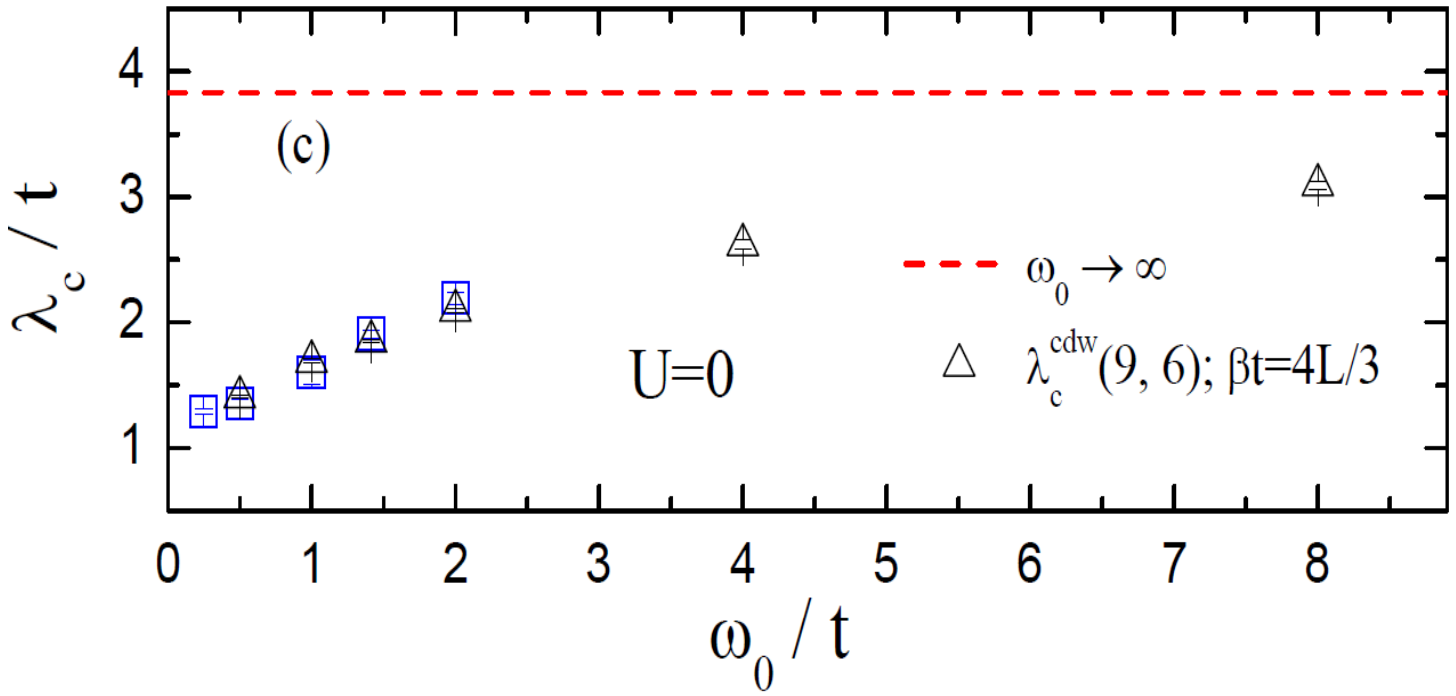

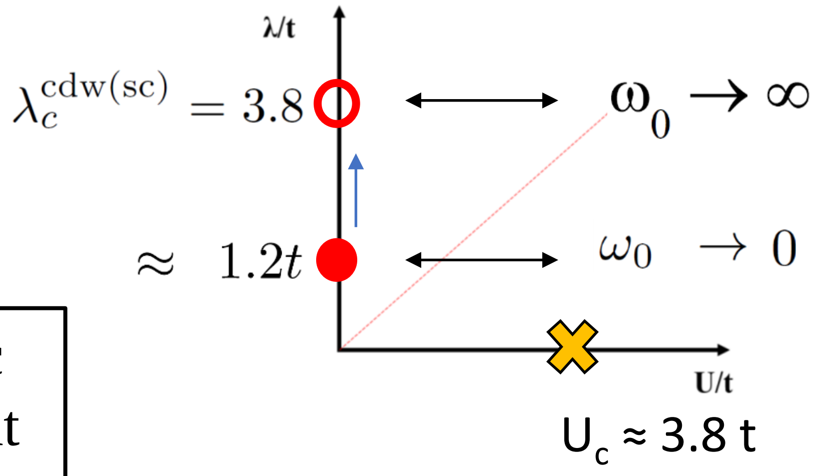

The *true* antiadiabatic limit seems to occur at very large values of ω

The Hubbard-Holstein model (U=λ)

AFQMC Method

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$U = \lambda$

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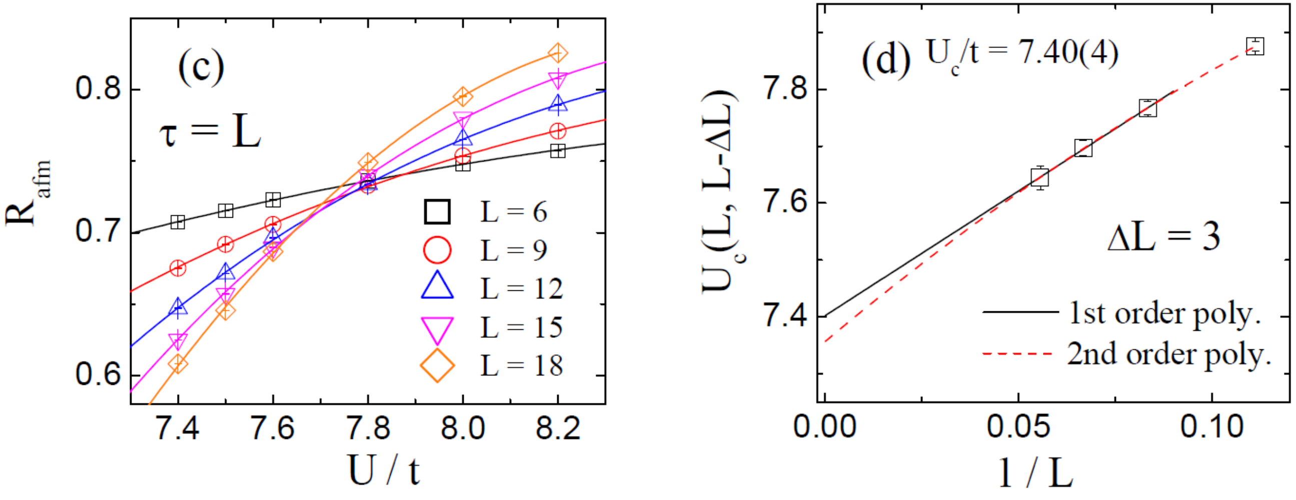

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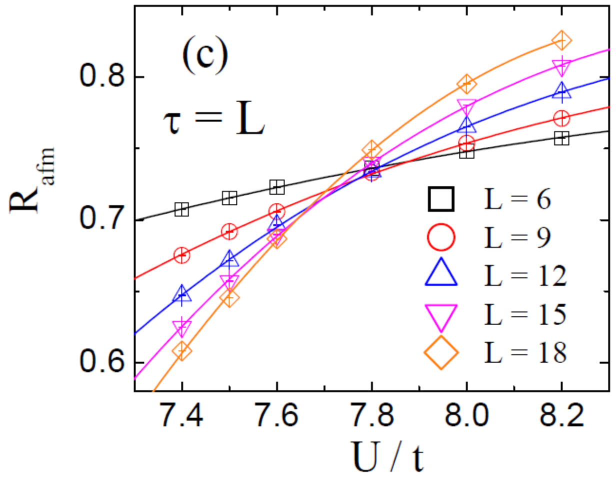

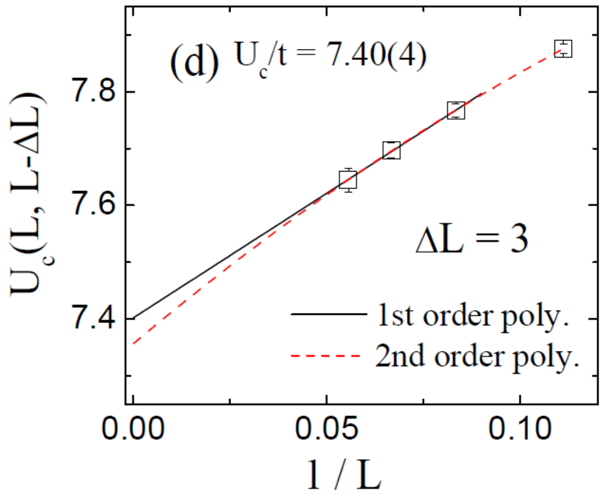

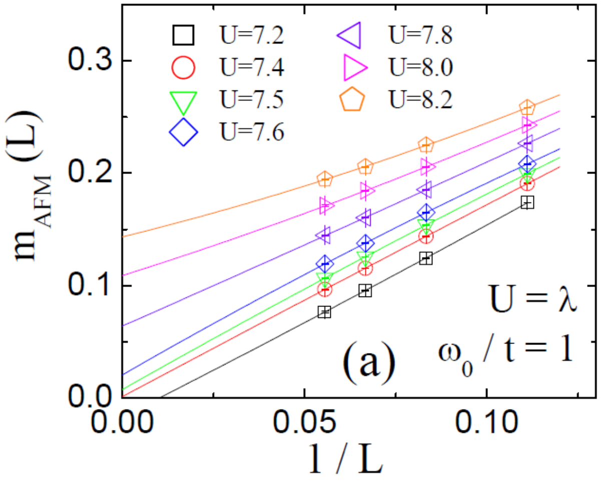

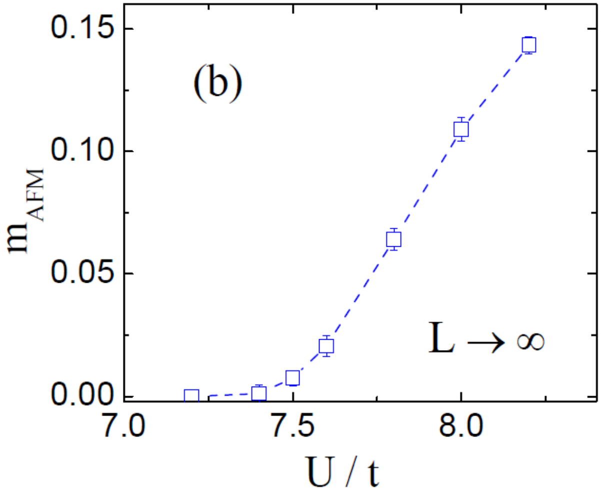

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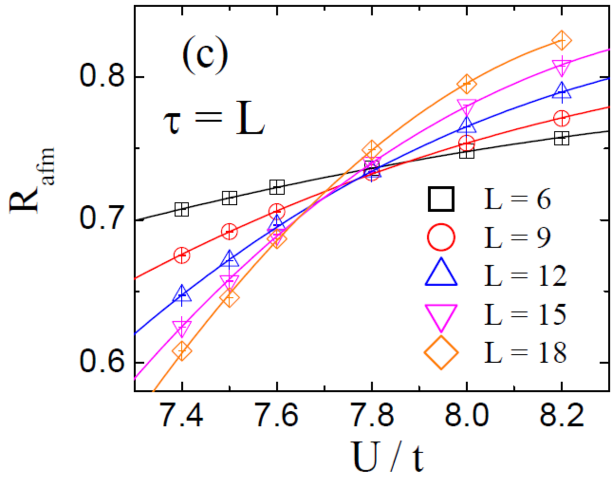
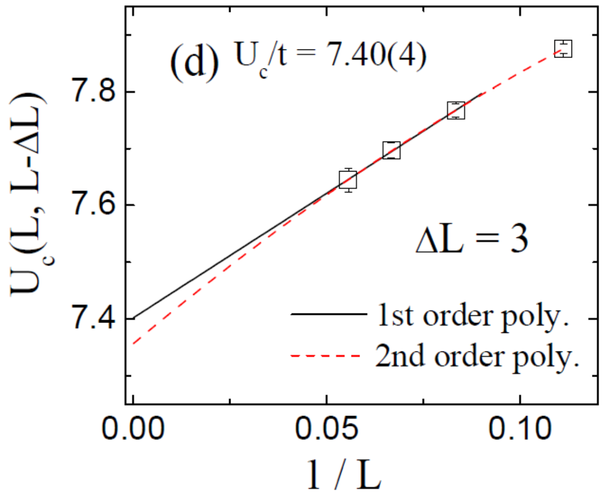
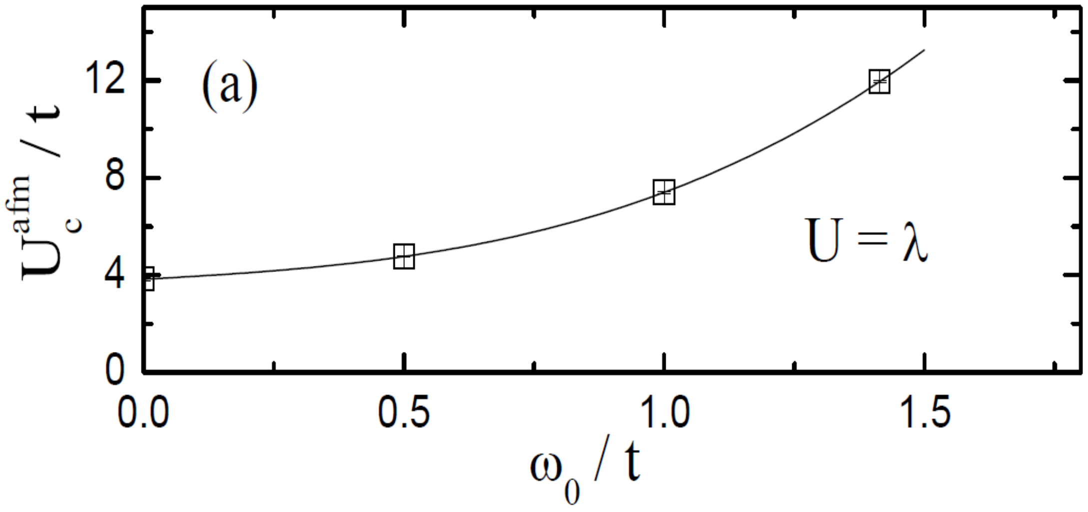
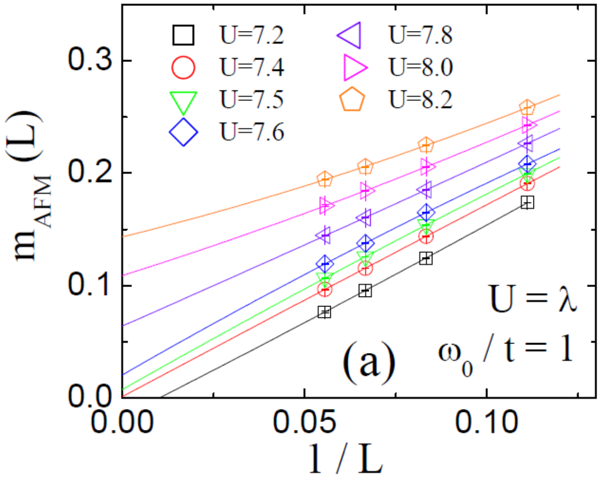
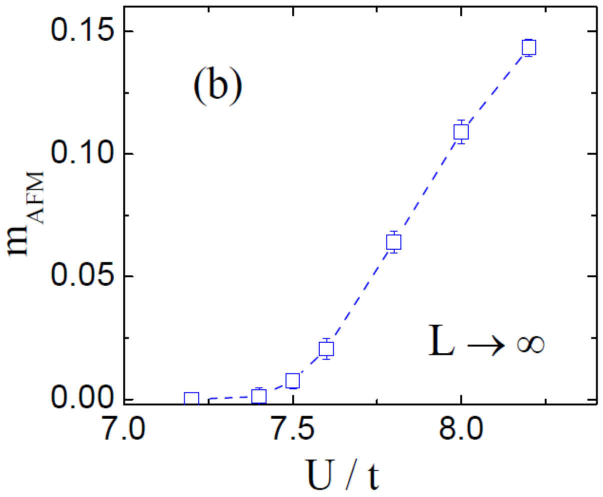
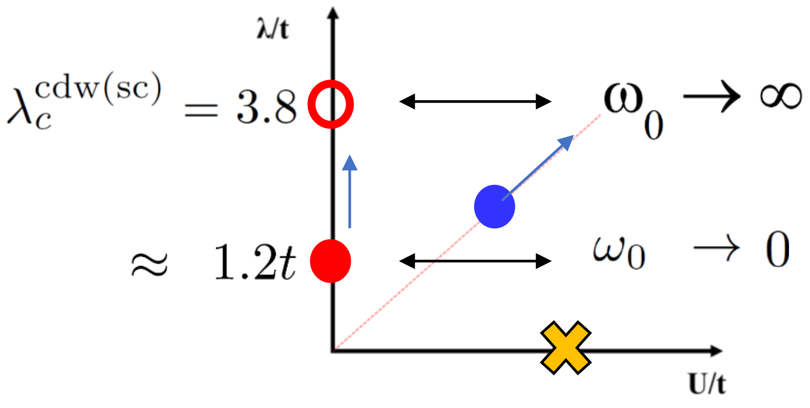








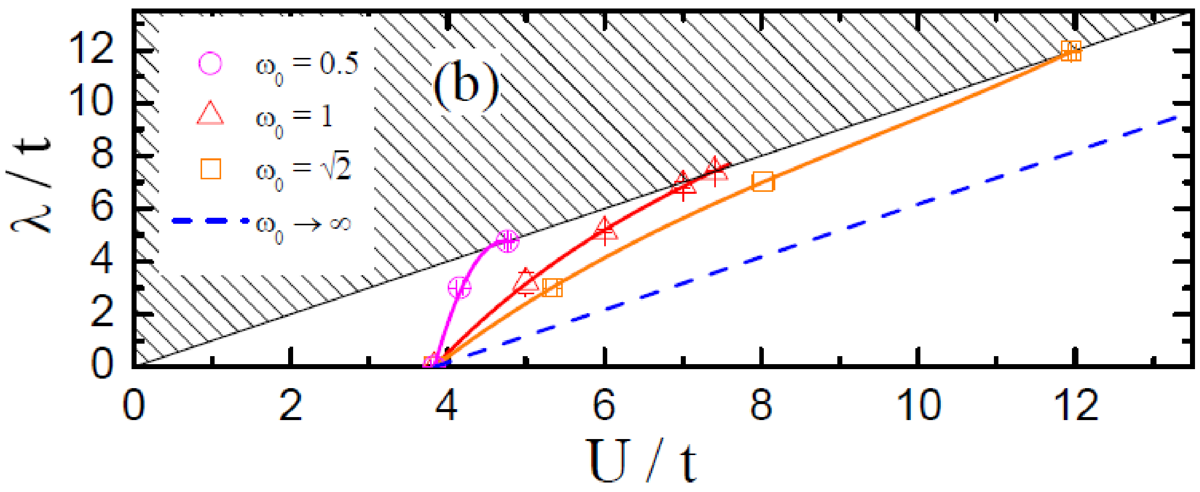




$U_c \approx 3.8\ t$

The Hubbard-Holstein model (U≠λ)

AFQMC Method



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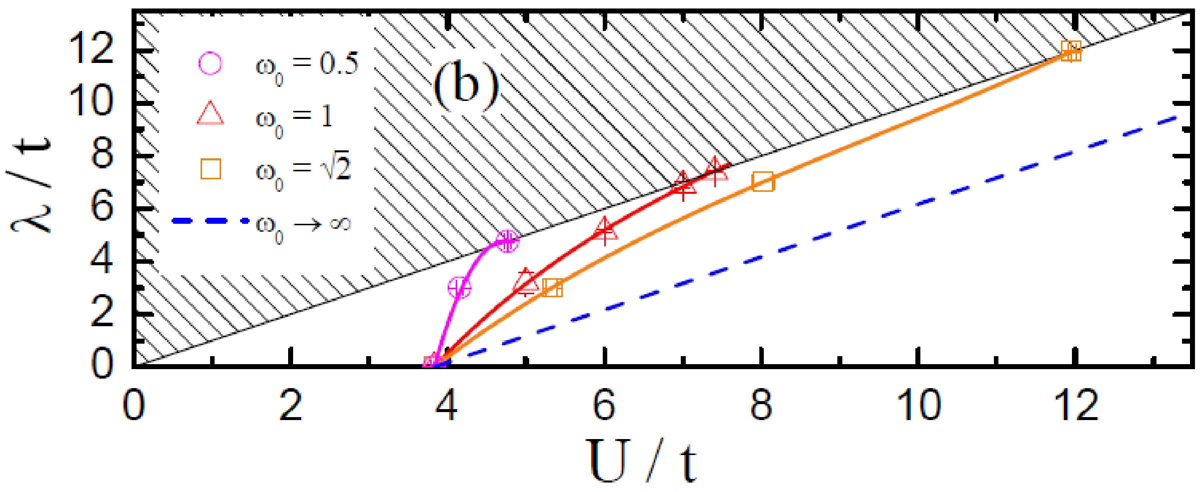
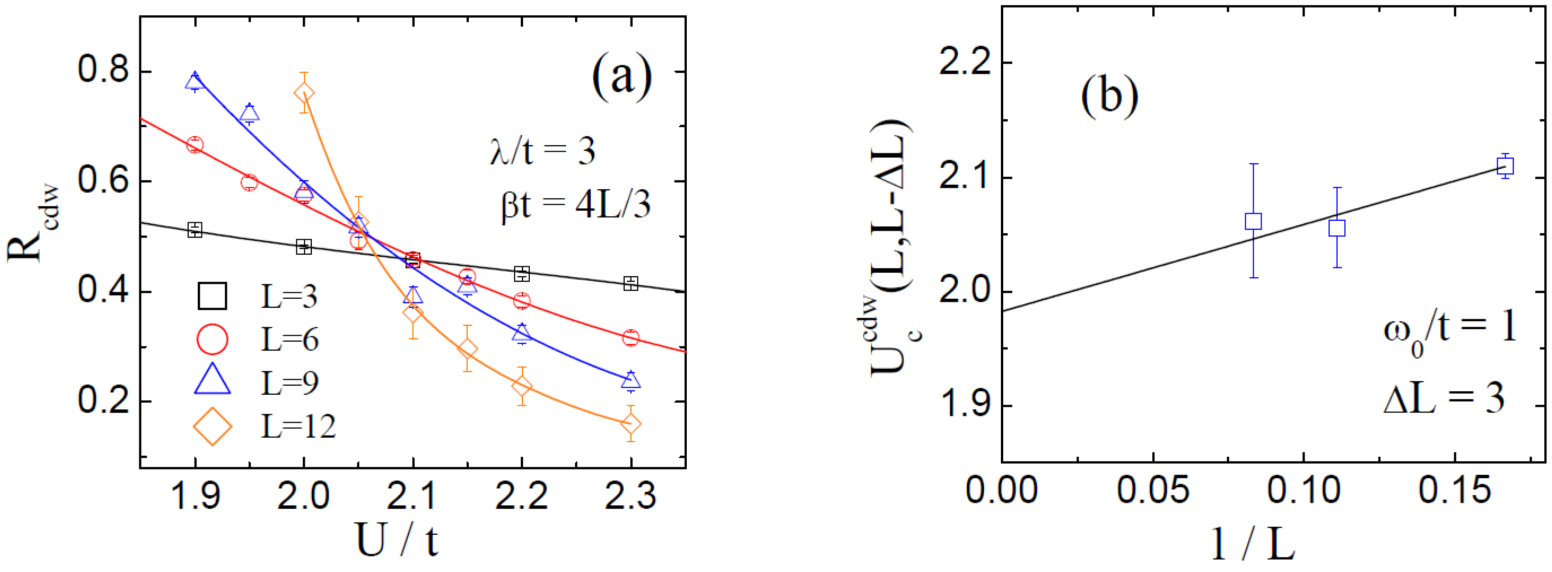


DQMC Method

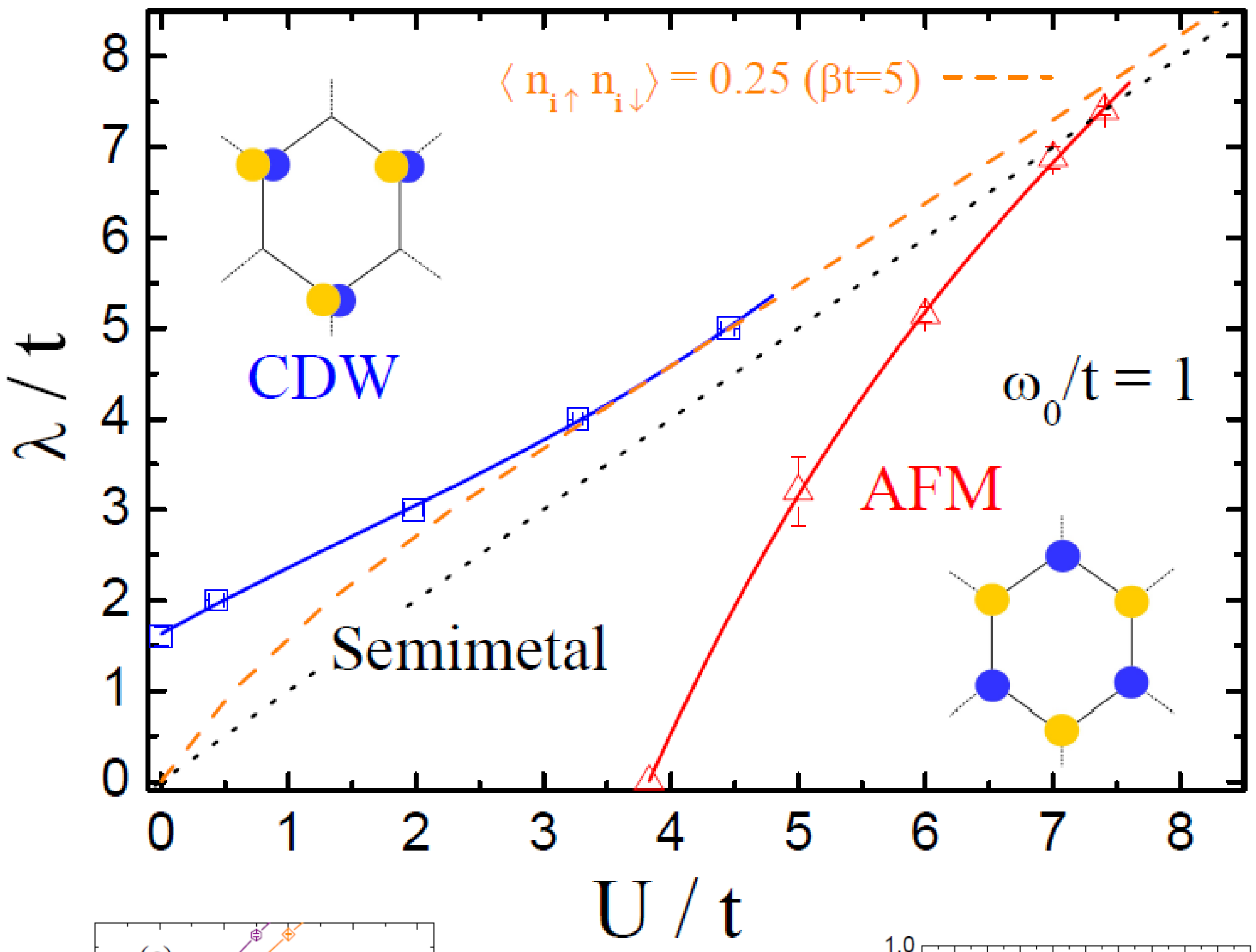
$\omega_0/t = 1$

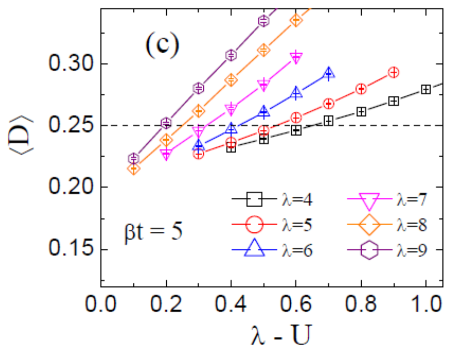
$\lambda/t = 3$

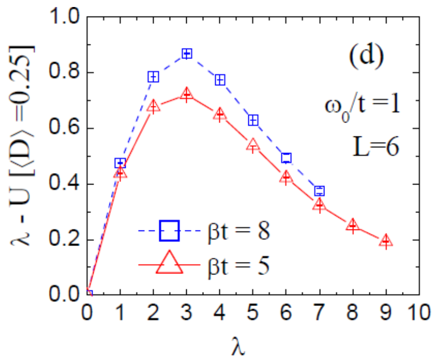
$U_c^{\mathrm{cdw}}/t \;=\; 1.98(7)$



The phase diagram of the Hubbard-Holstein model (honeycomb)







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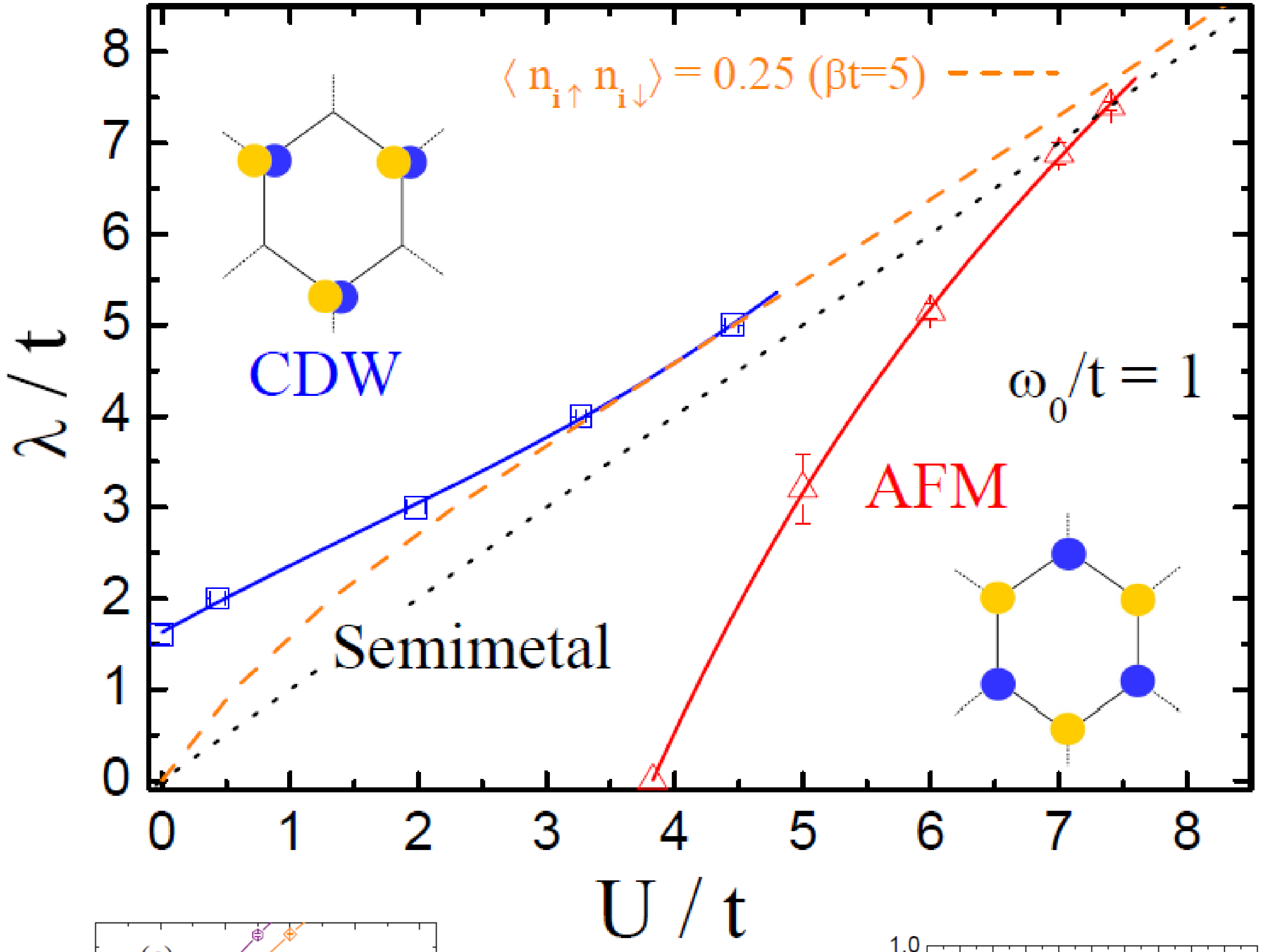

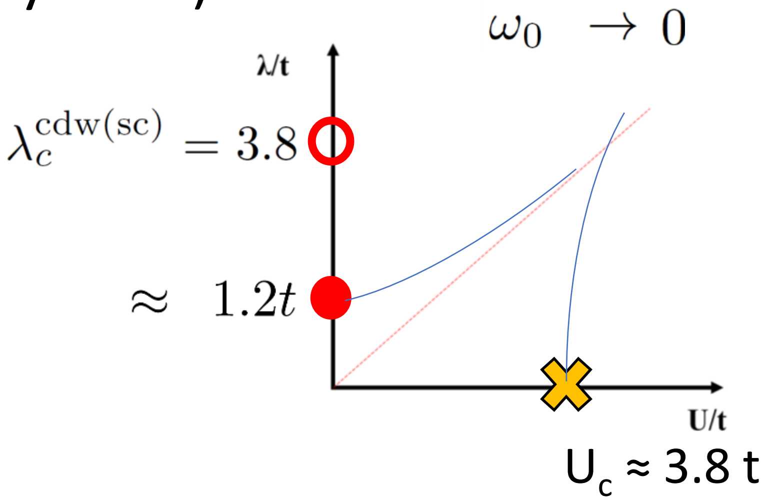

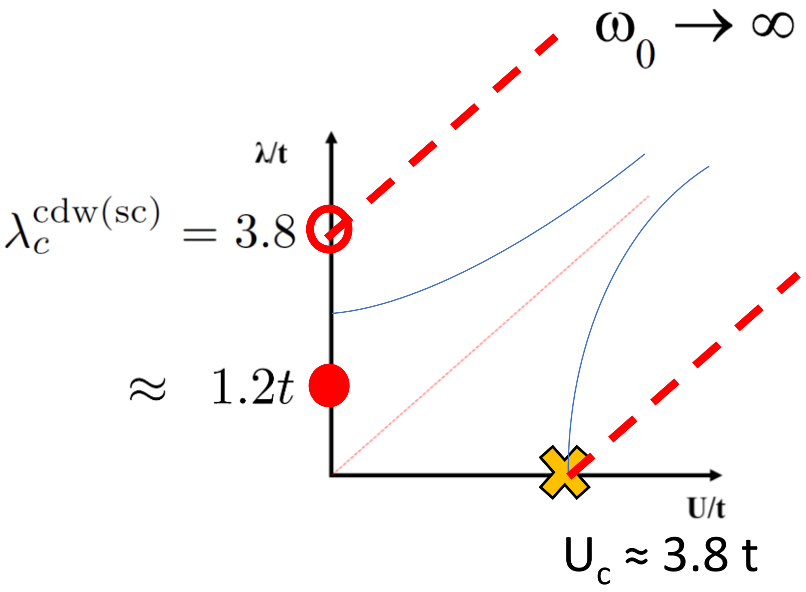

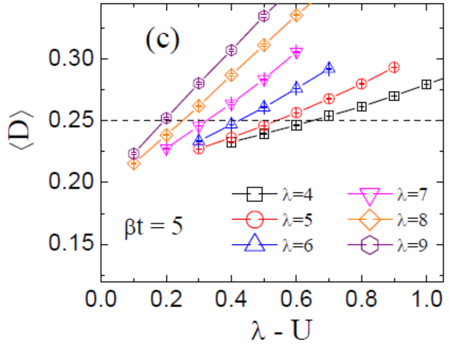

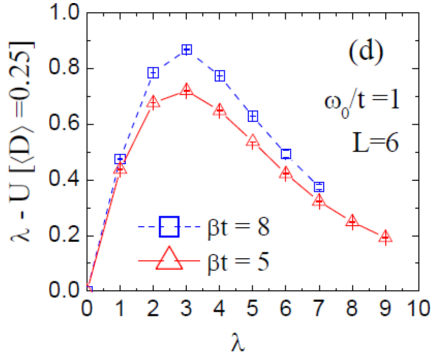

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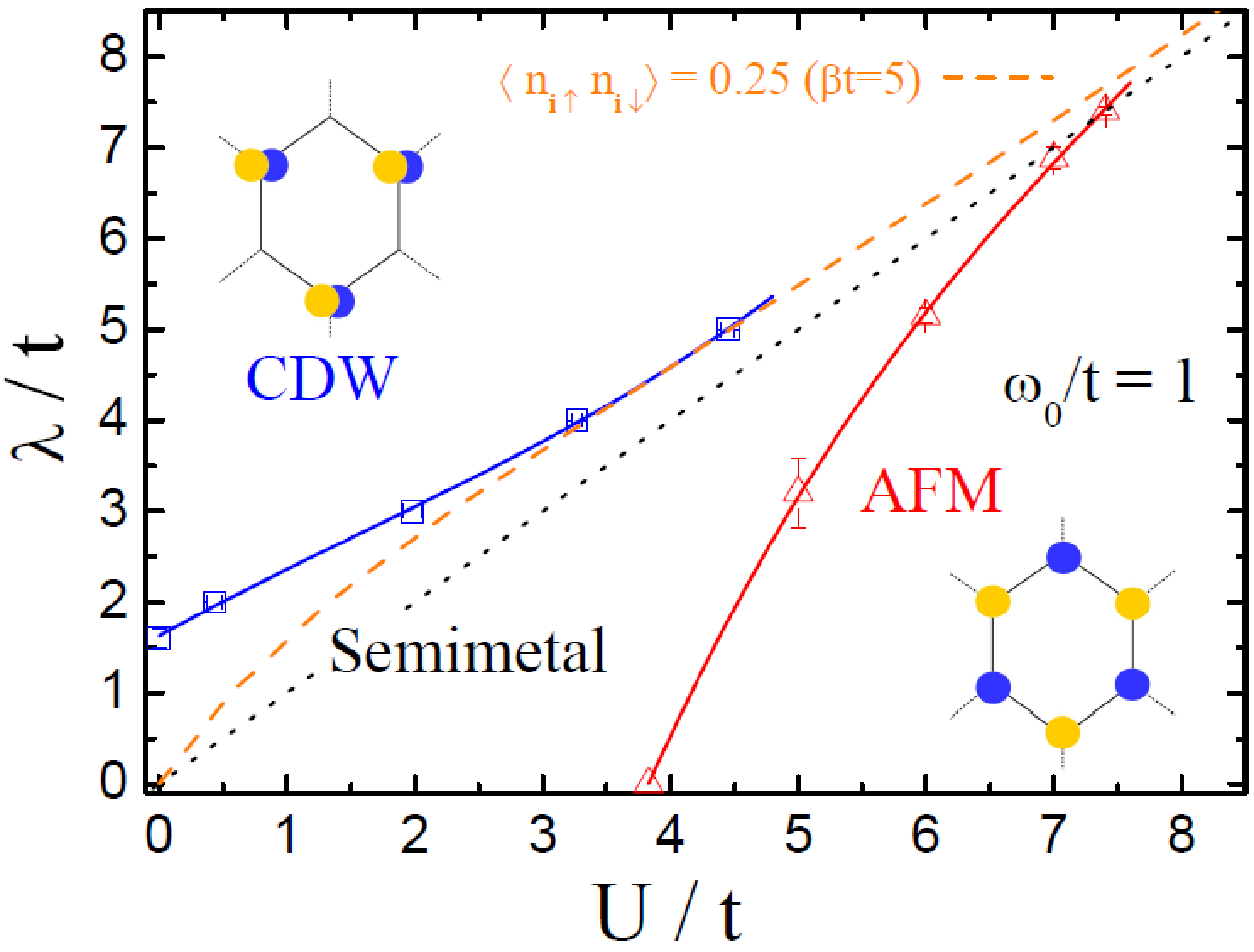

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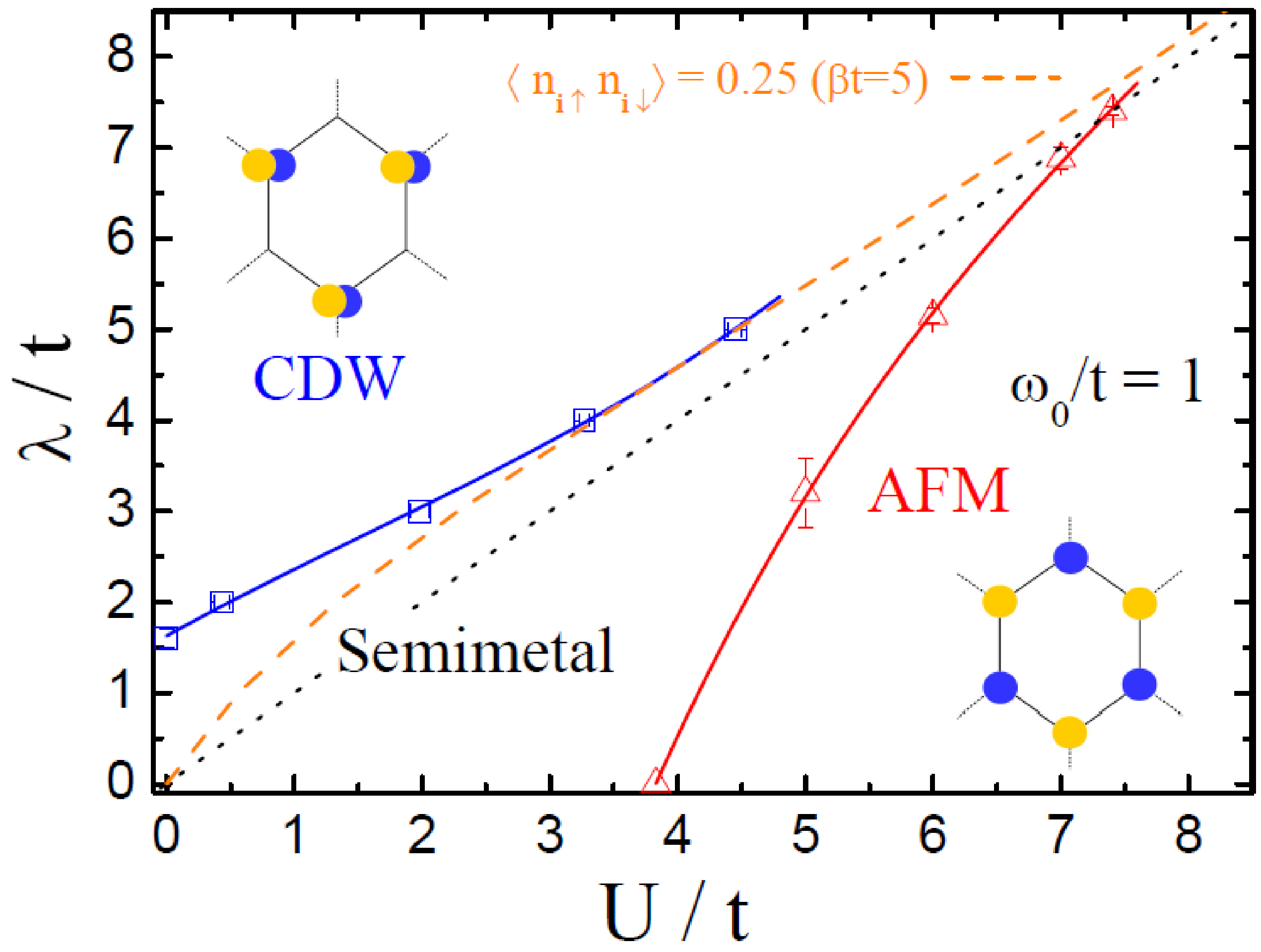
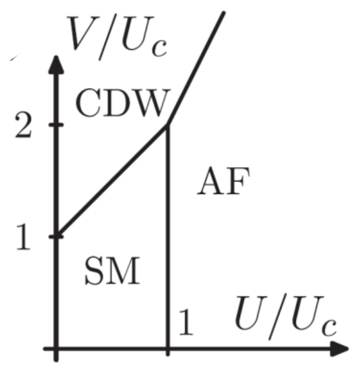
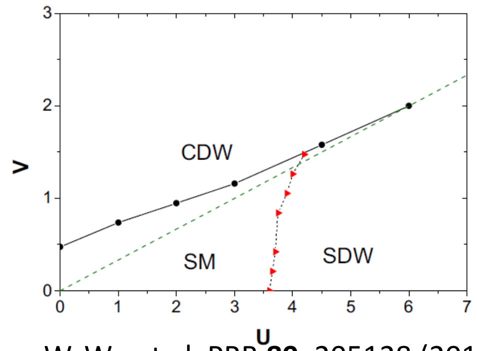


Extended Hubbard model

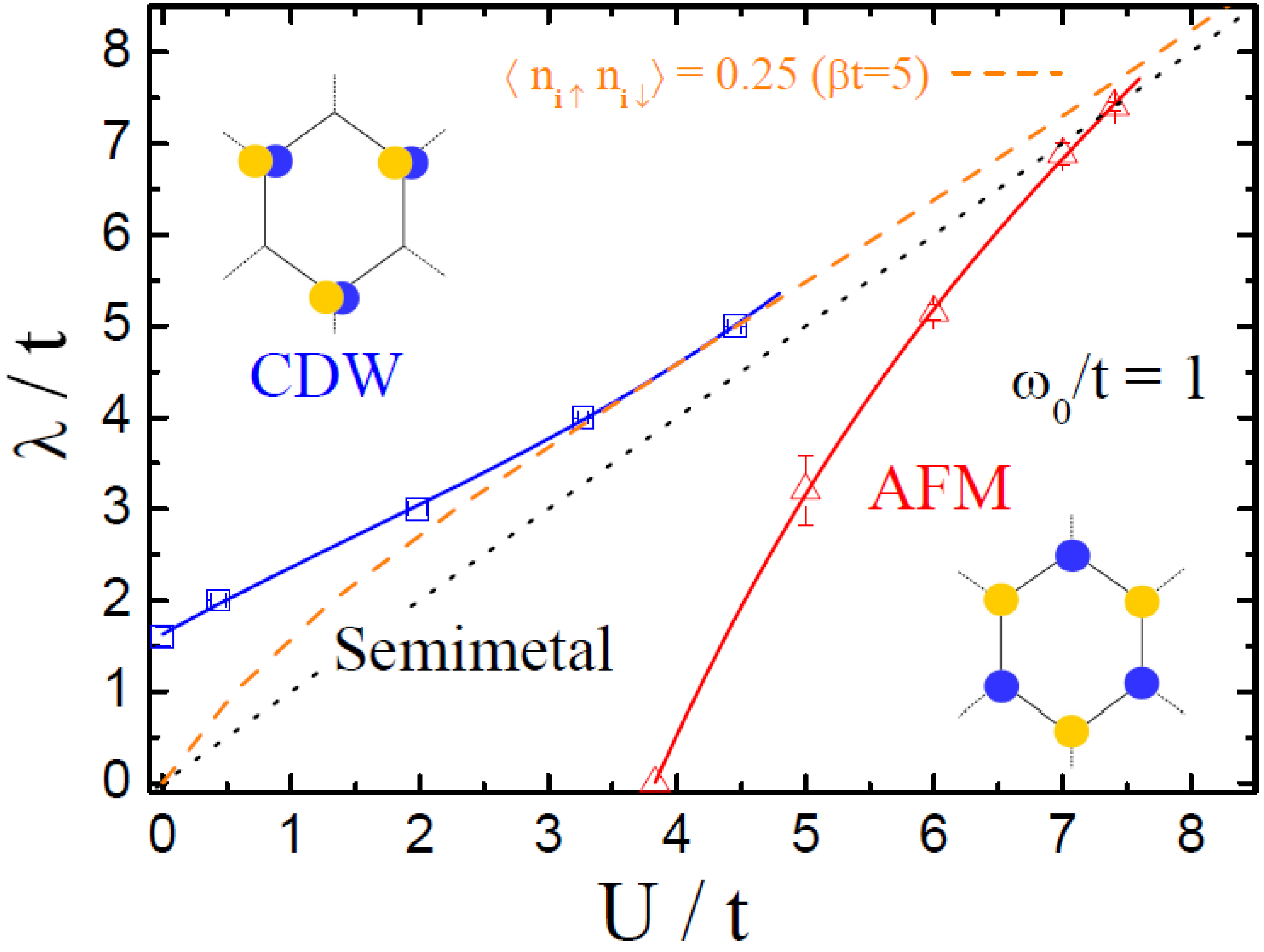


I. Herbut, PRL **97**, 146401 (2006)

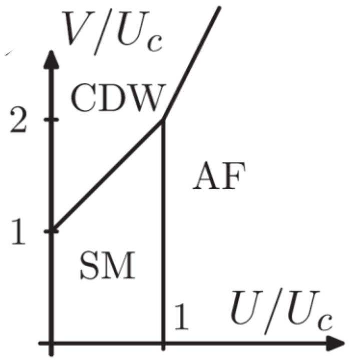


W. Wu et al, PRB **89**, 205128 (2014)

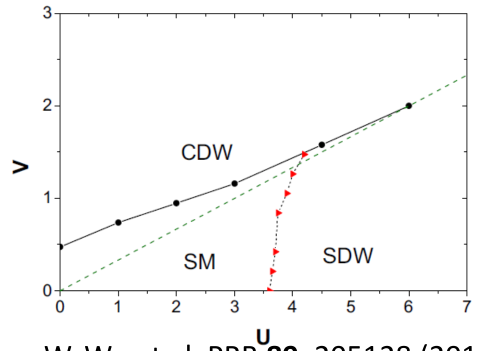
The phase diagram of the Hubbard-Holstein model (honeycomb)



Extended Hubbard model

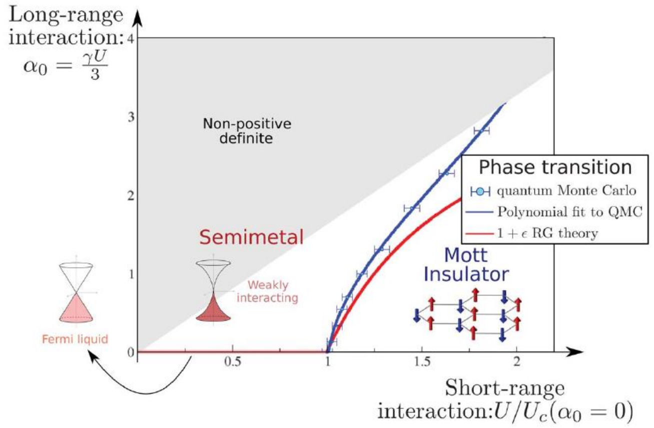


I. Herbut, PRL **97**, 146401 (2006)



W. Wu et al, PRB **89**, 205128 (2014)

Long-range interacting Hubbard model



H-K Tao et al, Science **361**, 570 (2018)

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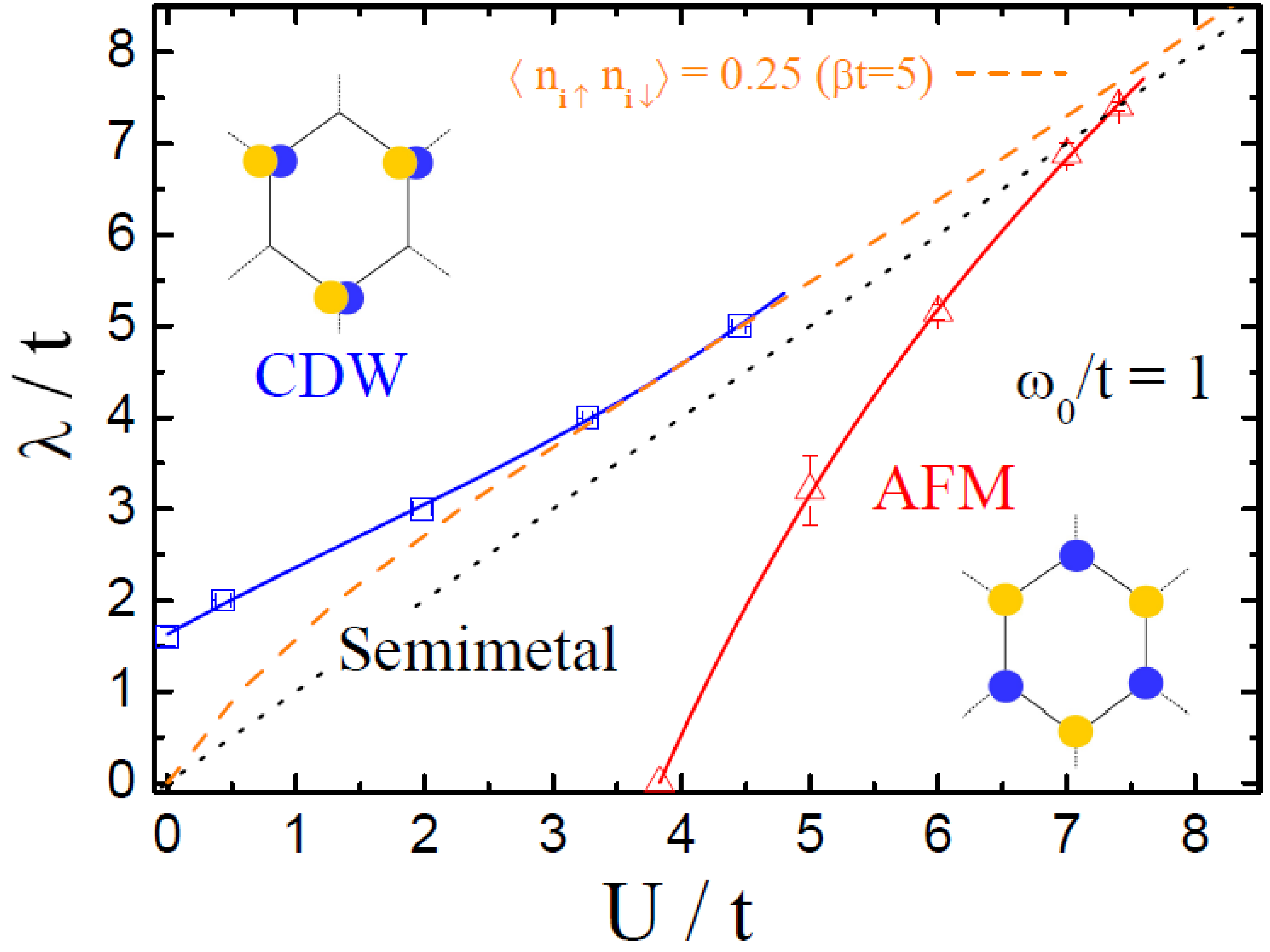
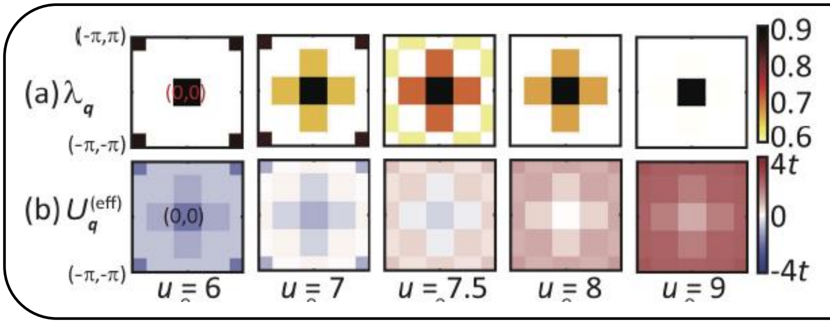
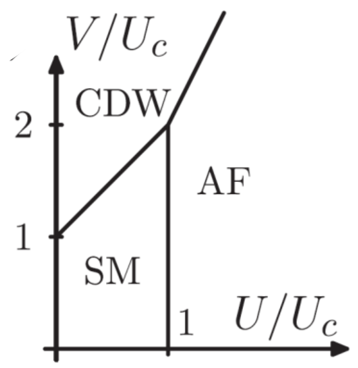




$U \approx \lambda$

Y. Wang et al,
ArXiv:1910.01792 (2019)

Extended Hubbard model



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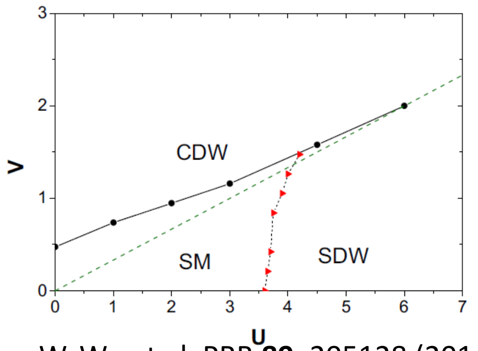

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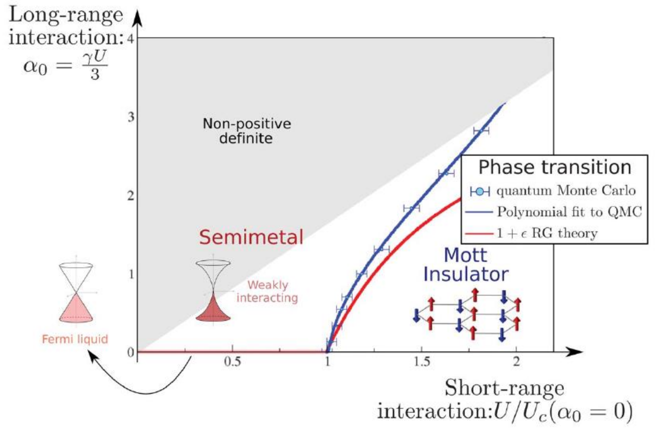

H-K Tao et al, Science **361**, 570 (2018)

Partial Conclusions

- Complete description of the QCPs of pure Holstein model;
- Existence of a metal-AFM transition on the line $U=\lambda$, with its critical coupling strength depending on ω_0;
- First unbiased phase diagram for the HHM in the honeycomb lattice, presenting its dependence with ω_0;

Magnetism and charge order in the honeycomb lattice

Natanael C. Costa,[1,2,*] Kazuhiro Seki,[3] and Sandro Sorella[1]

[1]*International School for Advanced Studies (SISSA), Via Bonomea 265, 34136, Trieste, Italy*
[2]*Instituto de Física, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro RJ, Brazil*
[3]*Computational Quantum Matter Research Team, RIKEN, Center for Emergent Matter Science (CEMS), Saitama 351-0198, Japan*

N. Costa et al, ArXiv: 2009.05586 (2020)

Submitted for publication

Outline

- Introduction
  - Peierls Instability and CDW formation
  - Experimental motivation

- The model and methodology

- Results
  - CDW, AFM and paring in the square lattice

  - CDW and AFM in the honeycomb lattice

- Outlooks

Outlooks

- Away from half-filling;
- Frustration (next-nearest neighbor hopping);
- Momentum-dependent EPC;
- Spin-orbit interactions.


Thank you for
your attention!

Introduction

Peierls Instability

Kohn anomaly

$$\hbar^2 \ddot{Q}_{\mathbf{q}} = -\Big[[Q_{\mathbf{q}}, \mathcal{H}], \mathcal{H} \Big]$$

$$\ddot{Q}_{\mathbf{q}} = -\omega_{\mathbf{q}}^2 Q_{\mathbf{q}} - g \left(\frac{2\omega_{\mathbf{q}}}{\hbar} \right)^{1/2} \rho(\mathbf{q})$$

$$\rho(\mathbf{q}, T) = \chi_0(\mathbf{q}, T) g \left(\frac{2\omega_{\mathbf{q}}}{\hbar} \right)^{1/2} Q_{\mathbf{q}}$$

$$\tilde{\omega}_{\mathbf{q}}^2(T) = \omega_{\mathbf{q}}^2 \left(1 - \frac{4 g_{\mathbf{q}}^2}{\hbar \omega_{\mathbf{q}}} \chi_0(\mathbf{q}, T) \right)$$

Introduction

Peierls Instability

X. Zhu et al., *Proc. Natl Acad. Sci. USA* **112**, 2367–2371 (2015)

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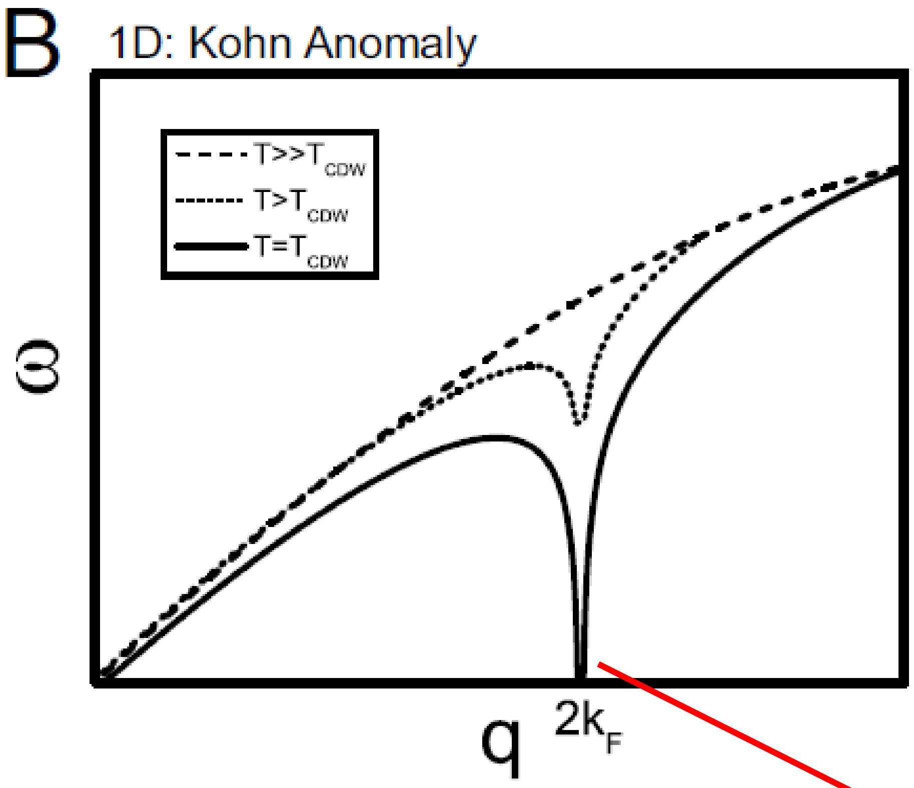


$$\tilde{\omega}(\vec{q}_{\text{nesting}})^2 < 0$$

Permanent deformation on the lattice

Introduction

Peierls Instability

Summary…

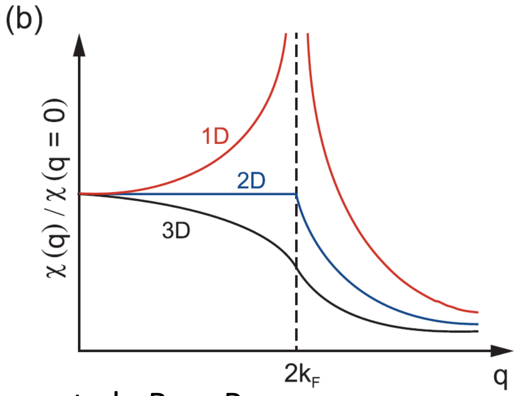
- Quasi-1D systems;
- Divergence on real and imaginary parts of electronic susceptibility (FSN);
- Metal-insulator transition at T_{CDW} ;
- Phonon softening at $\mathbf{q}=2\mathbf{k}_F$.

Introduction

The Nature of CDW

Criterion to CDW
(Perturbation theory)

$$\frac{4g_{\mathbf{q}}^2}{\hbar\omega_{\mathbf{q}}} > \frac{1}{\chi_0(\mathbf{q})}$$



C.-W. Chen et al., Rep. Prog. Phys. **79** 084505 (2016)

Ideal 1D Systems!

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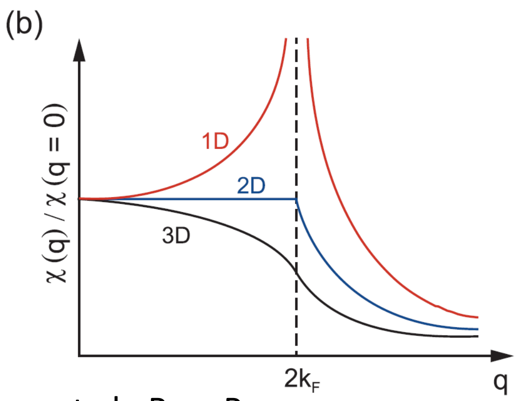

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Ideal 1D Systems!

- What if we do not have an ideal 1D system? ("bad nesting")
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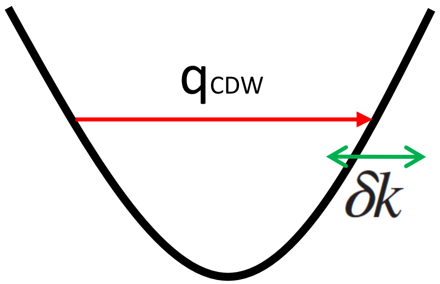

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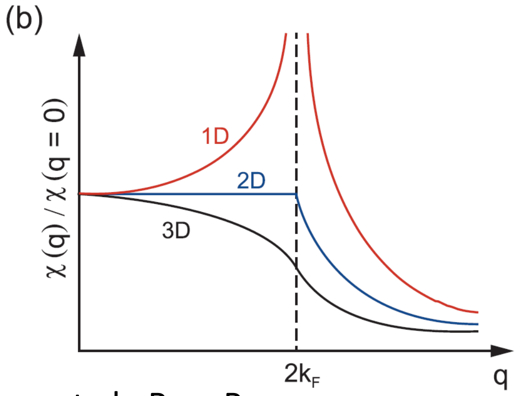

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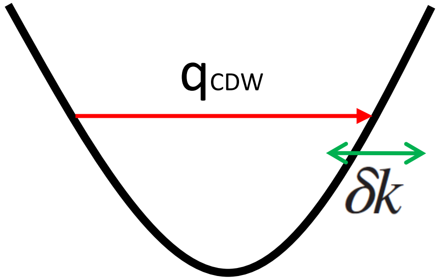
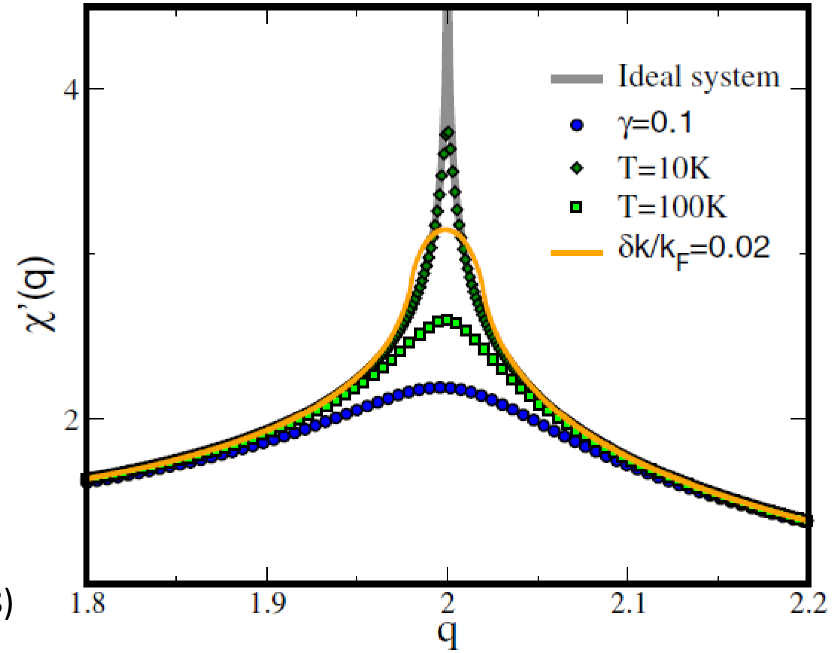


$$\chi'(q) = \frac{1}{2\delta k}\ln\left|\frac{q^2-(2k_F-\delta k)^2}{q^2+(2k_F-\delta k)^2}\right| + \frac{k_F}{\delta k q}\ln\left|\frac{(q-\delta k)^2-4k_F^2}{(q+\delta k)^2-4k_F^2}\right| + \frac{1}{2q}\ln\left|\frac{(q-2k_F)^2-\delta k^2}{(q+2k_F)^2-\delta k^2}\right|,$$



M.D. Johannes, I.I. Mazin, Phys Rev B **77** 165135 (2008)

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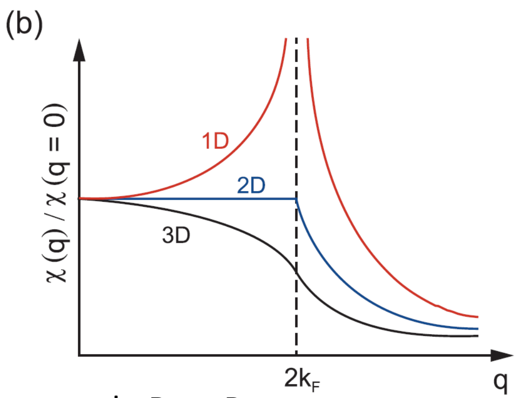

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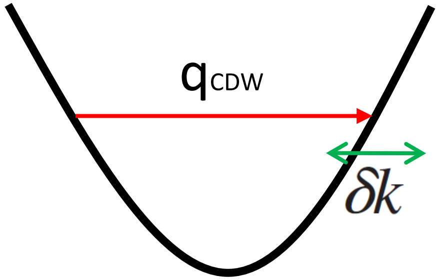

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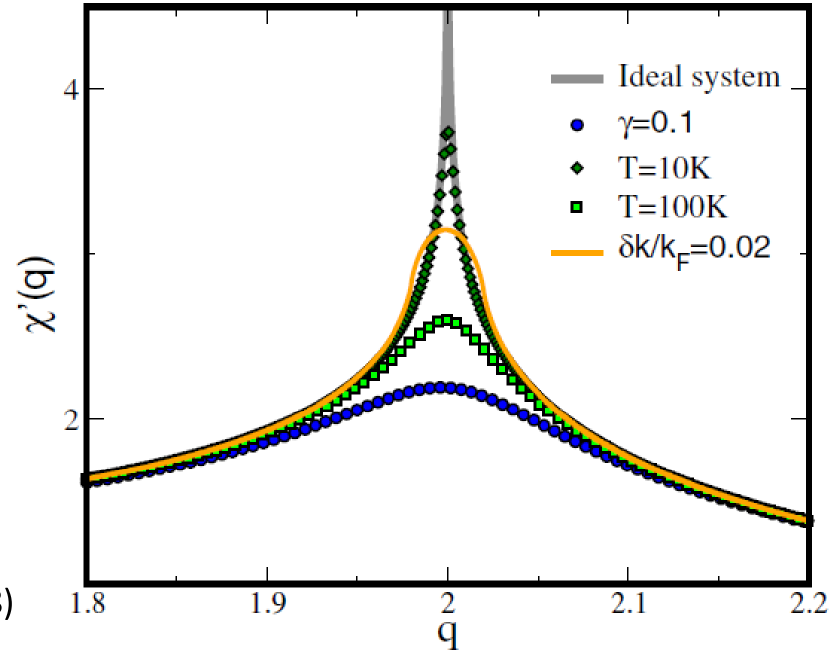
The electron-phonon coupling (EPC) and/or the phonon dispersion should play a central role in CDW formation!!



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