Metal-Insulator Transitions in 1D Electron System with next-nearest-neighbor hopping

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OUTLINE:

- **Motivations.**

- **Part I.**

  MI transition in the 1D $t - t'$ Hubbard Chain

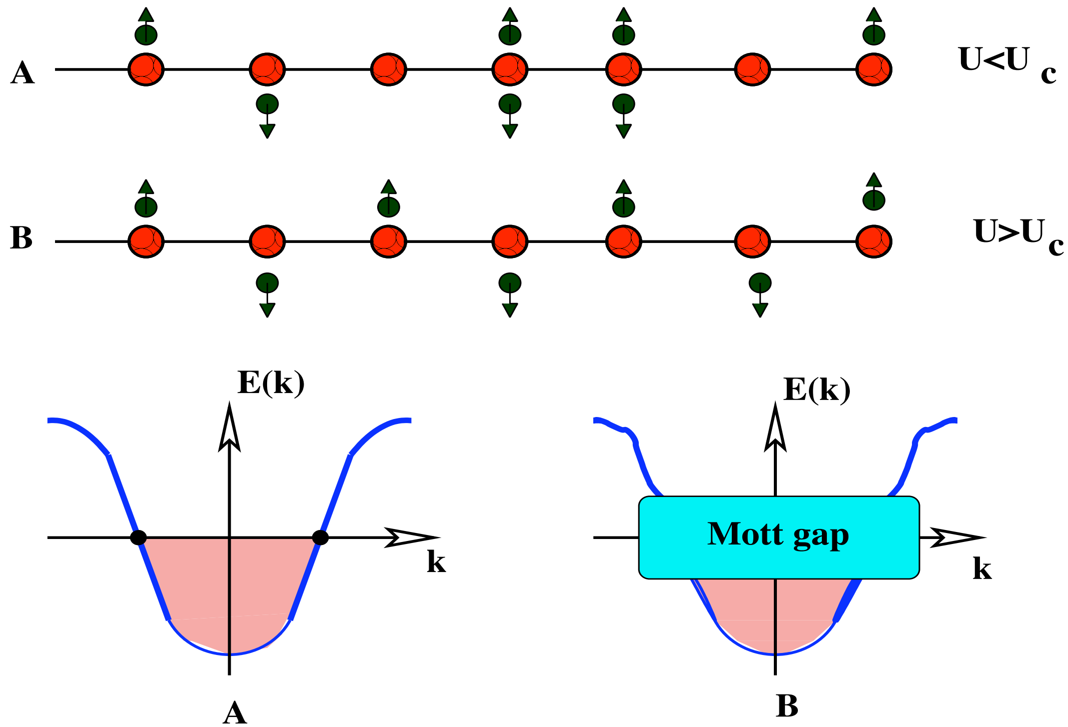
  GIJ, R.M. Noack and D.Baeriswyl, L. Tincani, PRB 76, 115118 (2007).

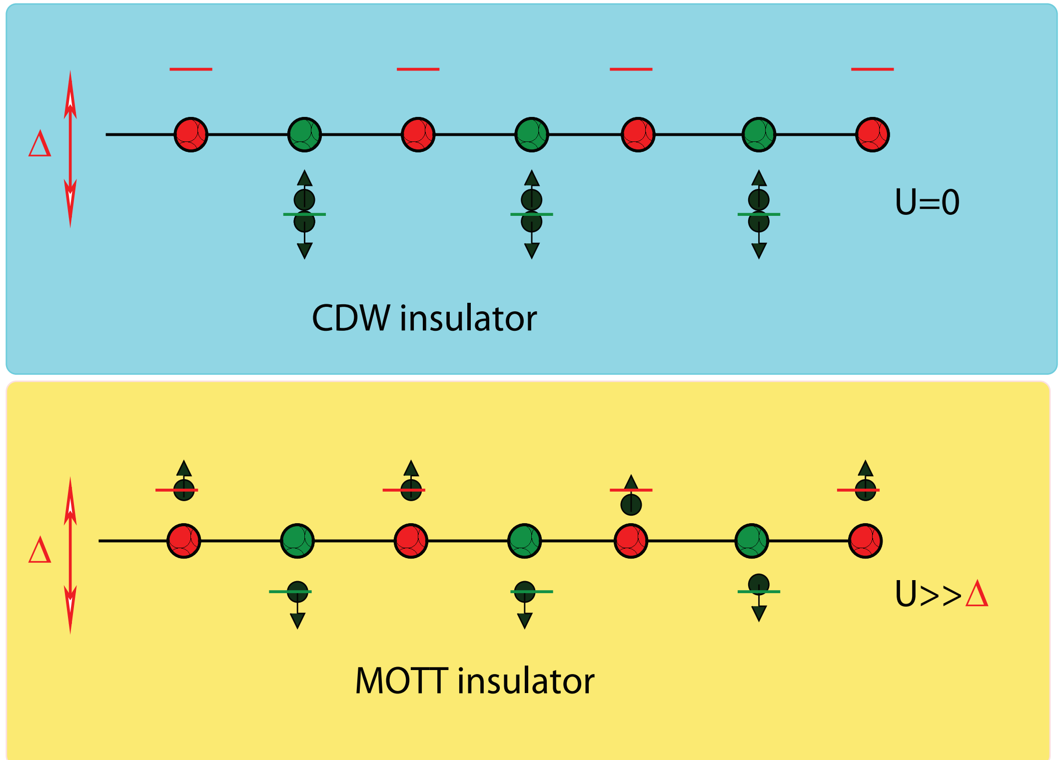
- **Part II.**

  MI transition in the 1D $t - t'$ Ionic Hubbard Chain

  GIJ, R. Hayn, P. Lombardo and E. Müller-Hartmann, PRB 75, 245122 (2007).

Mott Insulator





Band Insulator - Mott insulator transition.

From a BI to a Mott Insulator

Different routes:

the evolutionary way

F. Anfuso and A. Rosch, PRB **76**, 085124 (2007).

F. Anfuso and A. Rosch, PRB **75**, 142420 (2006).

via an intermediate insulating phase

M. Fabrizio, A. Gogolin and A.A. Nersesyan PRL, **83**, 2014 (1999)

M.E. Torio, A.A. Aligia, G.I.Japaridze and B. Normand, PRB **73**, 115109 (2006)

via an intermediate matallic phase

A. Garg, H. R. Krishnamurthy and M. Randeria, PRL **97**, 046403 (2006).

P. Lombardo, R. Hayn and G. I. Japaridze, PRB **74**, 085116 (2006).

2D square-lattice: Cluster-DMFT

N. Paris, R. T. Scalettar, et.al., PRL **98**, 046403 (2007). - *via a metal*

S.S. Kancharla and E. Dagotto, PRL, **98**, 016402 (2007).- *via an insulator*

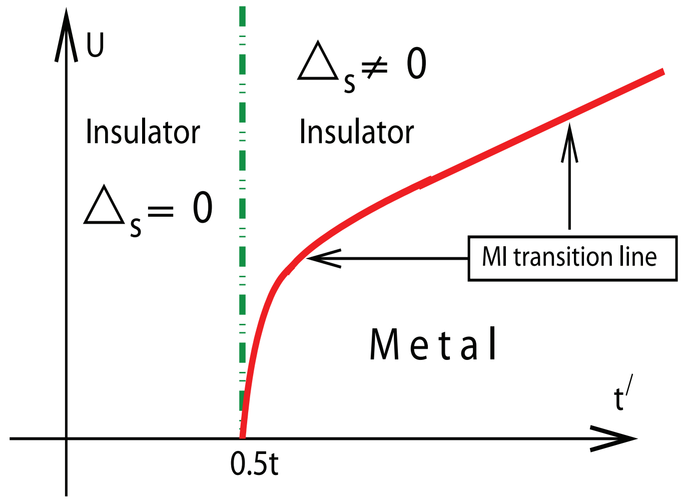
The Hamiltonian

$$
\begin{aligned}
\mathcal{H} = & -t \sum_{n,\sigma} \left(c^{\dagger}_{n,\sigma} c_{n+1,\sigma} + c^{\dagger}_{n+1,\sigma} c_{n,\sigma} \right) \\
& + t' \sum_{n,\sigma} \left(c^{\dagger}_{n,\sigma} c_{n+2,\sigma} + c^{\dagger}_{n+2,\sigma} c_{n,\sigma} \right) \\
& + \sum_{n,\sigma} \left(\delta\mu + (-1)^n \frac{\Delta}{2} \right) \rho_{n,\sigma} + U \sum_{n} \rho_{n,\uparrow} \rho_{n,\downarrow}
\end{aligned}
$$

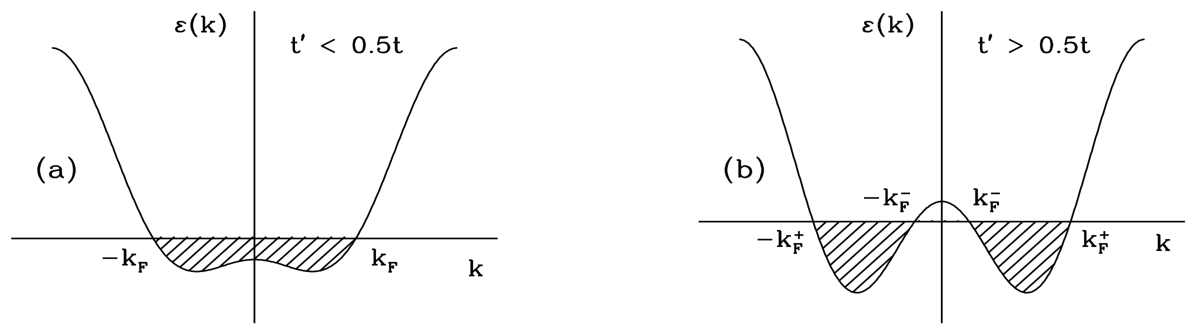
Limiting cases

- The Ionic chain: $U = 0$
- The Hubbard model: $t' = 0$ and $\Delta = 0$.
- The Ionic-Hubbard model: $t' = 0$
- The $t - t'$ Hubbard model: $\Delta = 0$

The $t - t'$ Hubbard chain



Qualitative phase diagram of the half-filled $t - t'$ Hubbard chain



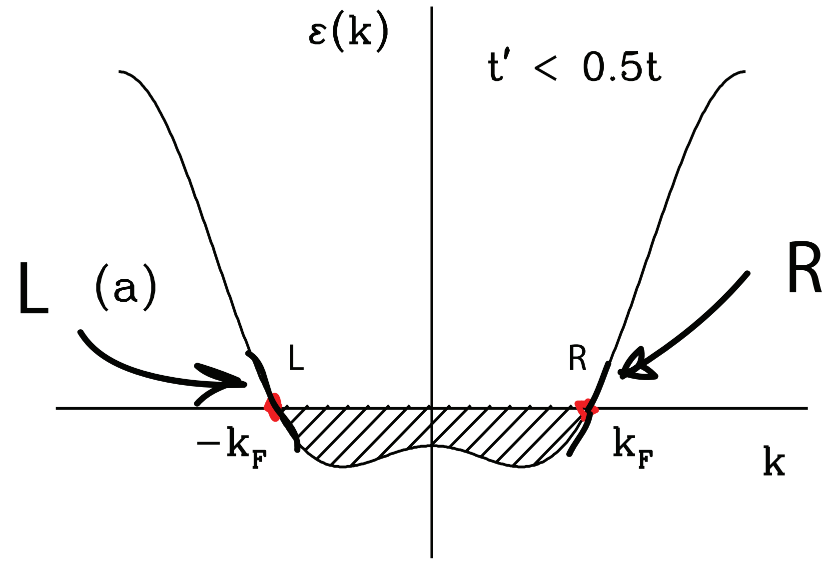
Dispersion relation $E(k)$ of the $t - t'$ chain

Change of the Topology of the Fermi-surface

The continuum-limit Hamiltonian

We start from the **2 Fermi points** picture:

$$c_{n,\sigma} \to e^{ik_F x}\psi_{R\sigma}(x) + e^{-ik_F x}\psi_{L\sigma}(x)$$



Here $\psi_{R\sigma}(x)$ and $\psi_{L\sigma}(x)$ describe the

Right-moving and Left-moving particles, respectively.

Using of this mapping gives:

A. Nearest-neighbor hopping term

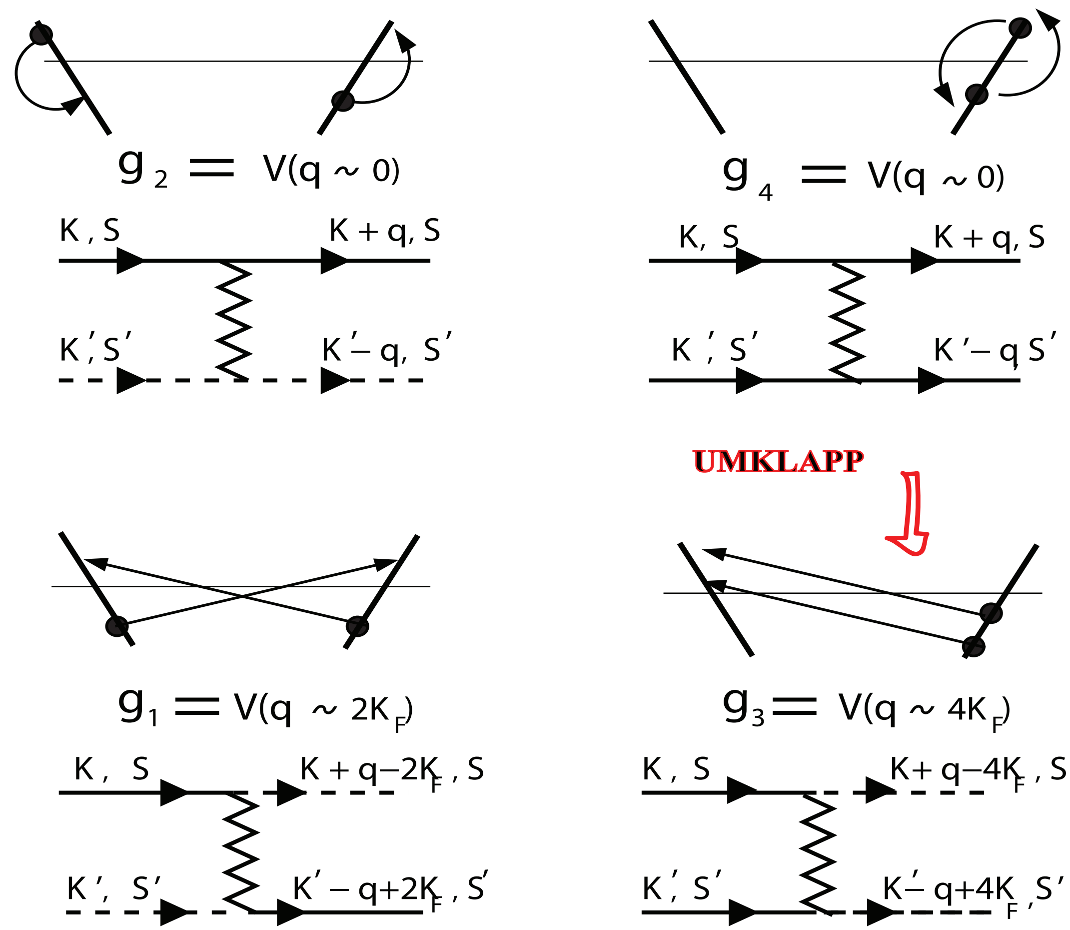
$$t \sum_n \left(c^\dagger_{n\sigma} c_{n+1\sigma} + c^\dagger_{n+1\sigma} c_{n\sigma} \right) \quad \Rightarrow$$
$$\Rightarrow \quad 2\, it \int dx \left(\psi^\dagger_{R\sigma}(x) \partial_x \psi_{R\sigma}(x) - \psi^\dagger_{L\sigma}(x) \partial_x \psi_{L\sigma}(x) \right)$$

B. The density operator

$$\sum_n \rho_{n,\sigma} = \sum_n c^\dagger_{n\sigma} c_{n\sigma} \quad \rightarrow$$
$$\rightarrow \int dx \left(\psi^\dagger_{R\sigma}(x) \psi_{R\sigma}(x) + \psi^\dagger_{L\sigma}(x) \psi_{L\sigma}(x) \right)$$

C. The Hubbard coupling

$$U \sum_n \rho_{n,\uparrow}\rho_{n,\downarrow} \quad \rightarrow$$



Bosonization and the Effective Theory

The R and L fermionic fields can be bosonized:

$$\psi_{R\sigma}(x) = \frac{1}{\sqrt{2\pi a_0}} e^{i\sqrt{\pi/2}[(\phi_c(x)+\theta_c(x))+\sigma(\phi_s(x)+\theta_s(x))]}$$

$$\psi_{L\sigma}(x) = \frac{1}{\sqrt{2\pi a_0}} e^{-i\sqrt{\pi/2}[(\phi_c(x)+\theta_c(x))+\sigma(\phi_s(x)+\theta_s(x))]},$$

- The Hubbard model: $t' = 0$ and $\Delta = 0$.

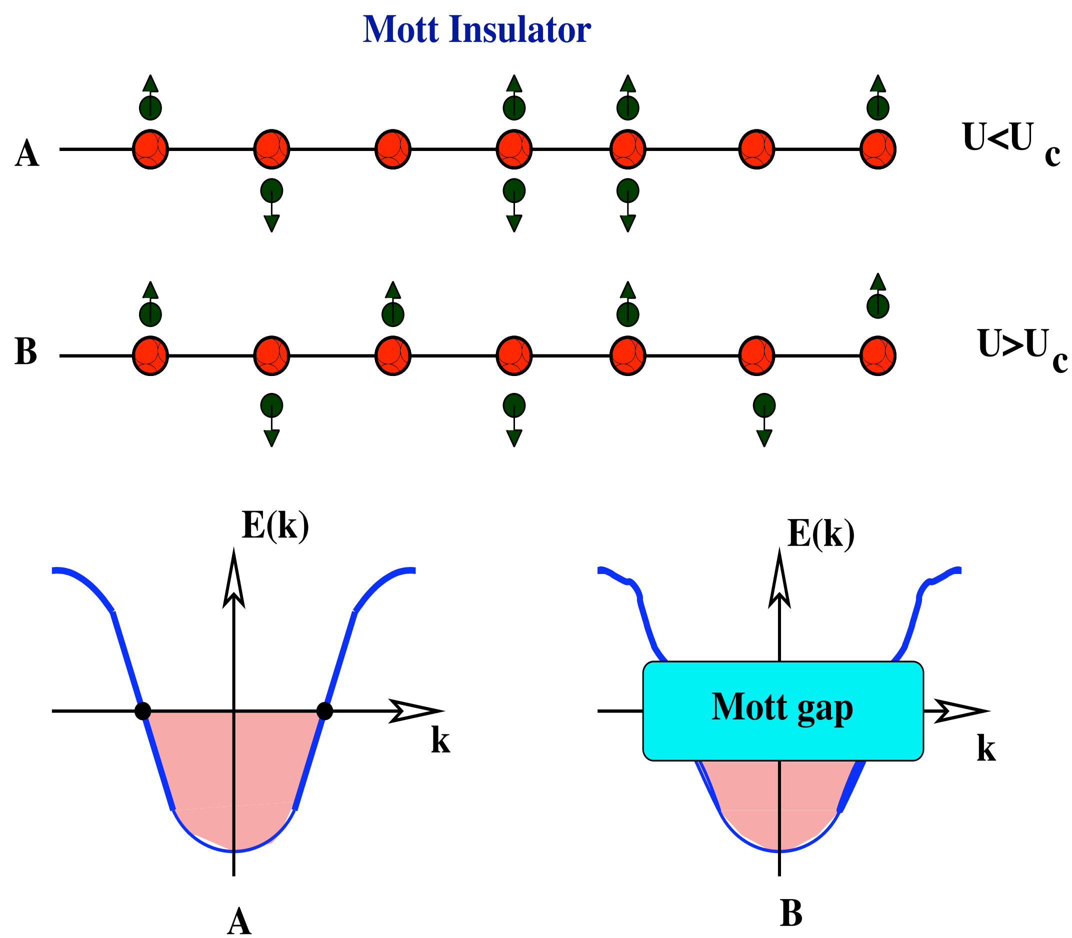
$$\mathcal{H} = H_s + H_c\,,$$

$$H_s = \frac{v_s}{2}\left[(\partial_x\varphi_s)^2 + (\partial_x\vartheta_s)^2\right]$$

$$H_c = \frac{v_c}{2}\left[(\partial_x\varphi_c)^2 + (\partial_x\vartheta_c)^2\right] - \frac{U}{2\pi\alpha^2}\cos(\sqrt{8\pi}\varphi_c)$$

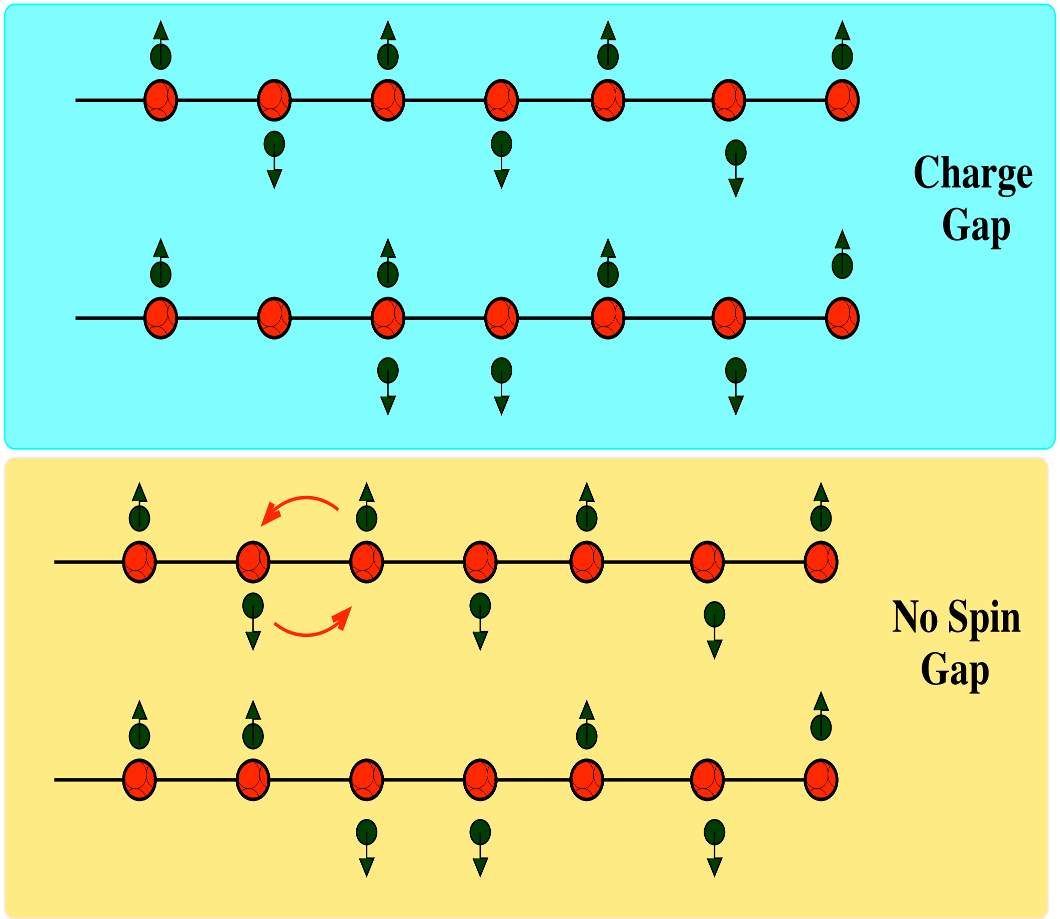
At half filling and for $U > 0$
the relevant cosine term determines mass in the charge SG.

Therefore the half-filled repulsive Hubbard model describes an *insulator* *with gapless spin excitation spectrum*



The MOTT INSULATOR!

Spin-Charge separation!



- **The $t - t'$ Hubbard model**: $\Delta = 0$

$$\mathcal{H} = -t \sum_{n,\sigma} \left(c^\dagger_{n,\sigma} c_{n+1,\sigma} + c^\dagger_{n+1,\sigma} c_{n,\sigma} \right)$$
$$+t' \sum_{n,\sigma} \left(c^\dagger_{n,\sigma} c_{n+2,\sigma} + c^\dagger_{n+2,\sigma} c_{n,\sigma} \right)$$
$$+\mu_0 \sum_{n,\sigma} \rho_{n,\sigma} + U \sum_{n} \rho_{n,\uparrow} \rho_{n,\downarrow}$$

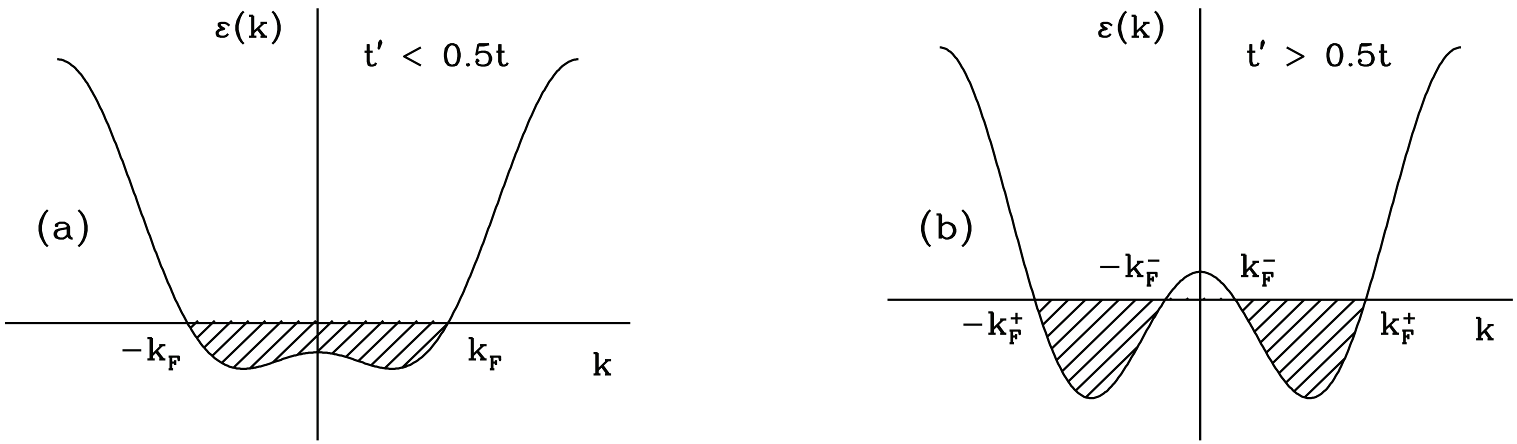
Next-Nearest-Neighbor hopping

$$t' \sum_n \left(c^\dagger_{n\sigma} c_{n+2\sigma} + c^\dagger_{n+2\sigma} c_{n\sigma} \right) \quad \Rightarrow$$
$$\Rightarrow \quad -2t' \int dx \left(\psi^\dagger_{R\sigma}(x) \psi_{R\sigma}(x + 2a_0) + \psi^\dagger_{L\sigma}(x) \partial_x \psi_{L\sigma}(x + 2a_0) \right)$$
$$-2t' \int dx \left(\psi^\dagger_{R\sigma}(x) \psi_{R\sigma}(x) + \psi^\dagger_{L\sigma}(x) \partial_x \psi_{L\sigma}(x) + \mathcal{O}(a_0) \right)$$

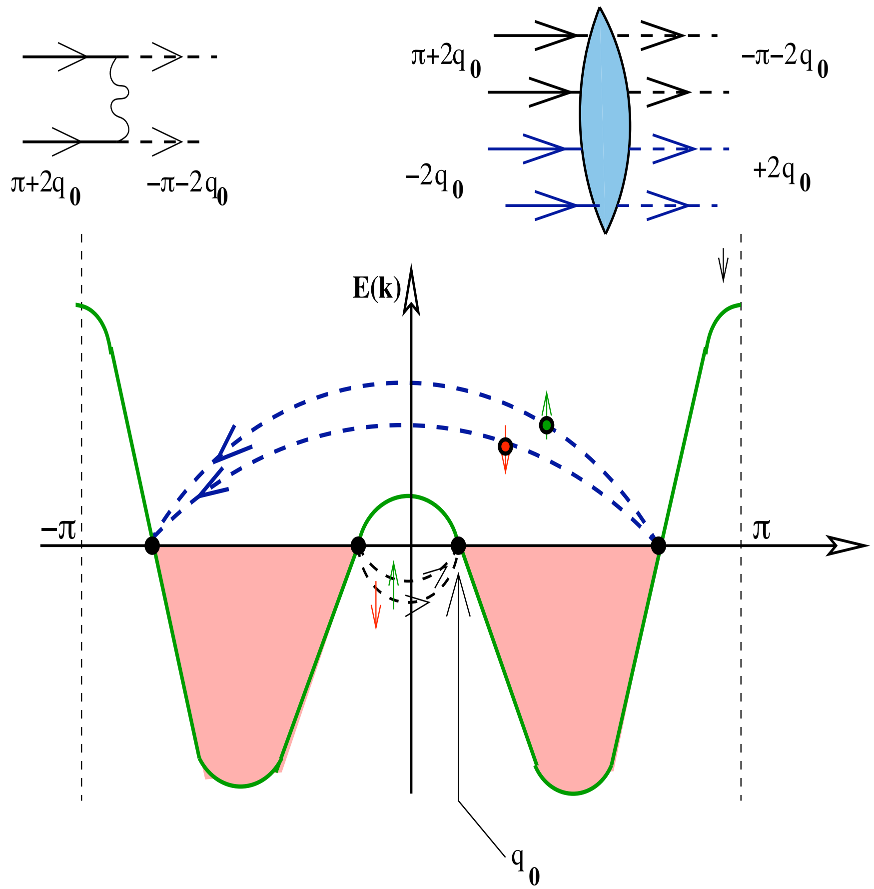
leads to

⇒ • **A. To the Renormalization of the Chemical Potential μ**

$$\mu_{\text{eff}} = \mu_0 - 2t' = \begin{cases} 0 & \text{for} \quad t' < 0.5t \\ \frac{t^2}{2t'} - 2t' \neq 0 & \text{for} \quad t' > 0.5t\,. \end{cases}$$



⇒ • **B. For $t' > 0.5t$ leads to Suppression of the Standard Umklapp Scattering**



$$H_c = \frac{v_c}{2}\left[(\partial_x\varphi_c)^2 + (\partial_x\vartheta_c)^2\right] - \frac{U}{2\pi\alpha^2}\cos(\sqrt{16\pi K_c}\varphi_c)$$

The Effective Theory at $t' \neq 0$,

$$\mathcal{H} = H_s + H_c\,,$$

$$H_s = \frac{v_s}{2}\left[(\partial_x\varphi_s)^2 + (\partial_x\vartheta_s)^2\right]$$

$$H_c = \frac{v_c}{2}\left[(\partial_x\varphi_c)^2 + (\partial_x\vartheta_c)^2\right] - \mu_{\text{eff}}\sqrt{\frac{\mathbf{2}}{\pi}}\partial_{\mathbf{x}}\varphi_{\mathbf{c}} - \frac{U}{2\pi\alpha^2}\cos(\sqrt{8\pi}\varphi_c)$$

where

$$\mu_{\text{eff}} = \begin{cases} 0 & \text{for} \quad t' < 0.5t \\ \frac{t^2}{2t'} - 2t' \neq 0 & \text{for} \quad t' > 0.5t\,. \end{cases}$$

H_c is the Hamiltonian of the Commensurate-incommensurate transition

A. A. Nersesyan and GIJ, JETF Pis'ma **27**, 356 (1978)
V. L. Pokrovsky and A. L. Talapov, Phys. Rev. Lett. **42**, 65 (1979);

$$H_c = \frac{v_c}{2}\left[(\partial_x\varphi_c)^2 + (\partial_x\vartheta_c)^2\right] - \mu_{\text{eff}}\sqrt{\frac{\mathbf{2}}{\pi}}\partial_{\mathbf{x}}\varphi_{\mathbf{c}} - \frac{U}{2\pi\alpha^2}\cos(\sqrt{8\pi}\varphi_c)$$

At $\mu_{eff} = 0$ and $U > 0$ the minimum of the energy is reached at

$$\varphi_c(x) = constant = \sqrt{2\pi}n, \qquad n = 0, \pm1, \pm2, ...$$

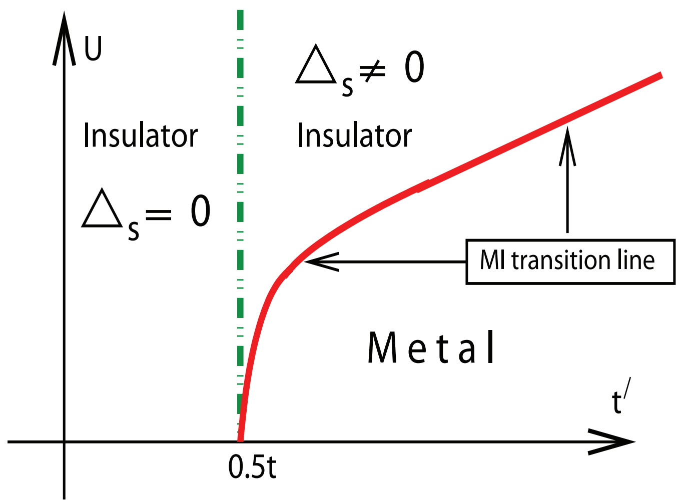
while at $U = 0$ and $\mu_{eff} \neq 0$ at $\partial_x\varphi_c(x) = constant$.

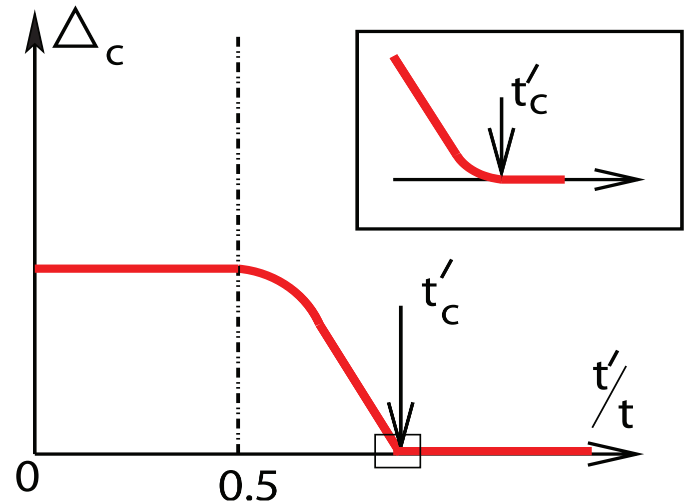
The charge density ,

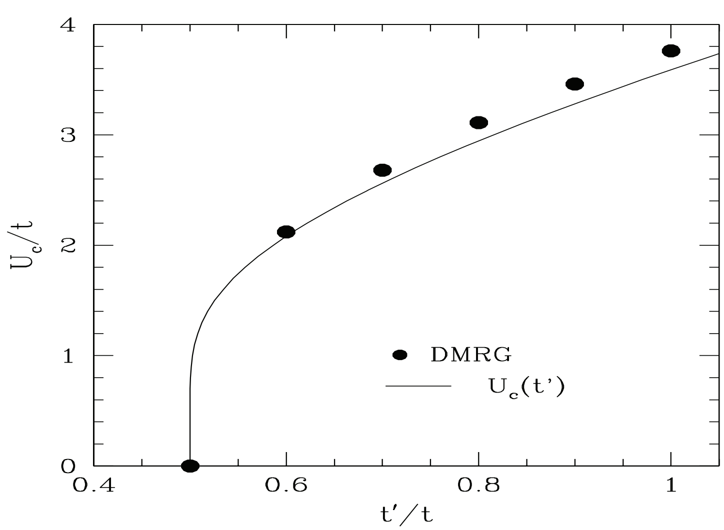
$$\begin{aligned} \rho_c(x) &\simeq \frac{1}{\sqrt{2\pi}}\partial_x\varphi_c + A_{4k_F}\cos(4k_F x)\cos(\sqrt{8\pi}\varphi_c) \\ &+ A_{2k_F}\cos(2k_F x)\sin(\sqrt{2\pi}\varphi_c)\cos(\sqrt{2\pi}\varphi_s) \end{aligned}$$

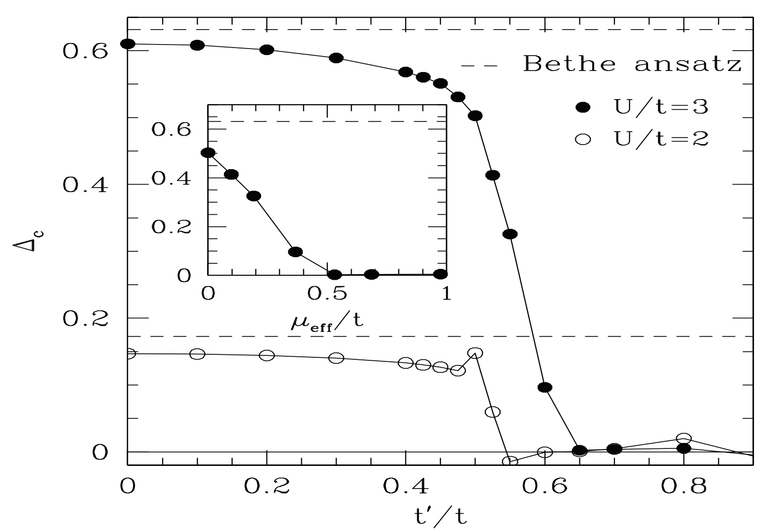
Pinning of the field φ_c **suppresses** the $2k_F$ charge fluctuations and stabilizes the 4 component. At 1/2-filling, $4k_F = 2\pi$ and therefore in the gapped (insulating) phase stror commensurate with lattice electron distribution - one electron per lattice unit, is realized.

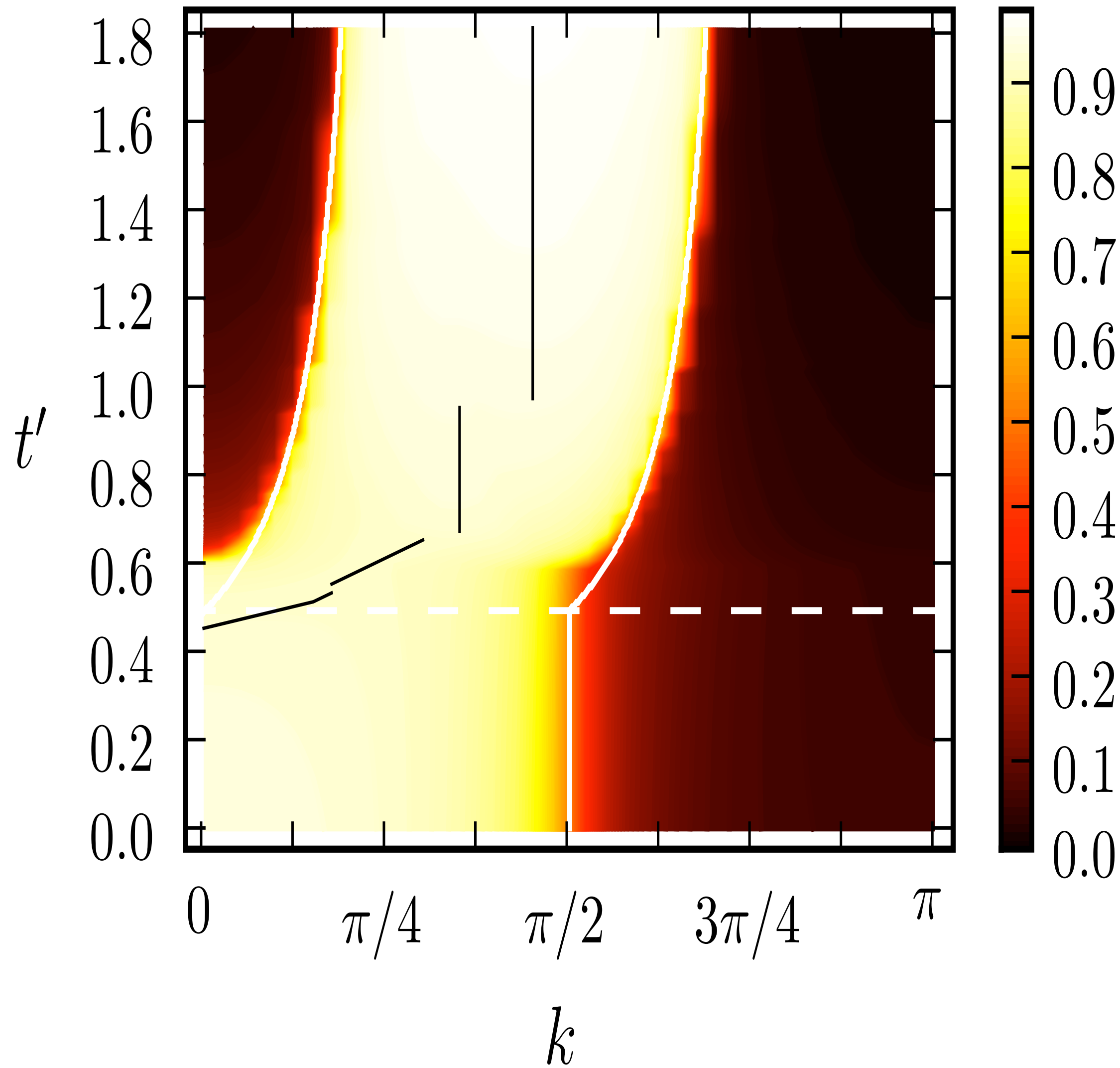
Competition between the chemical potential term and the condensation energy connec with gap drives a phase transition from a **gapped (insulating) phase** at $\mu_{eff} < \mu^c_{eff}$ a **gapless (metallic) phase** at $\mu_{eff} > \mu^c_{eff} = M_c$





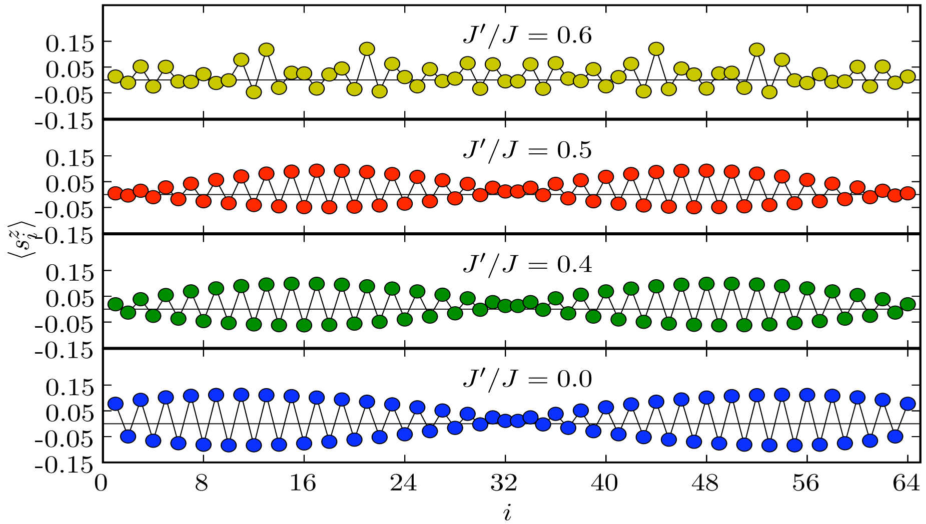


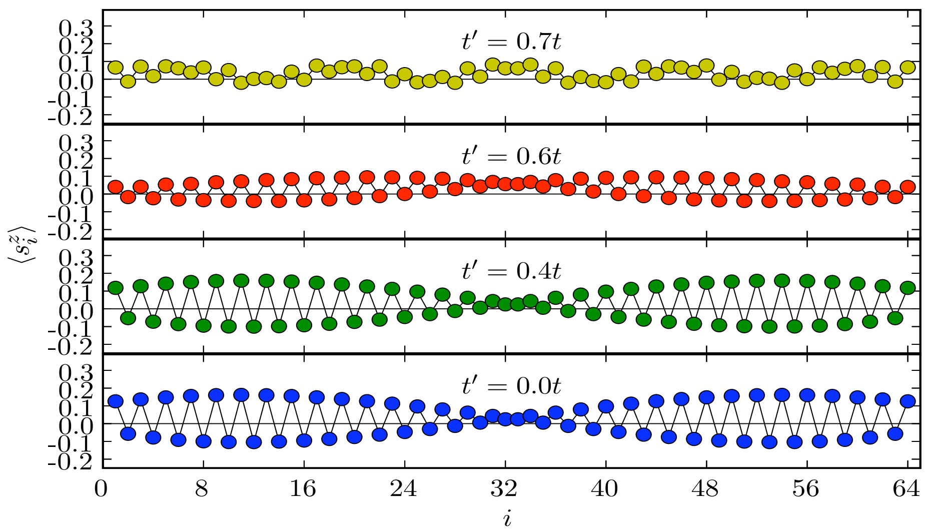




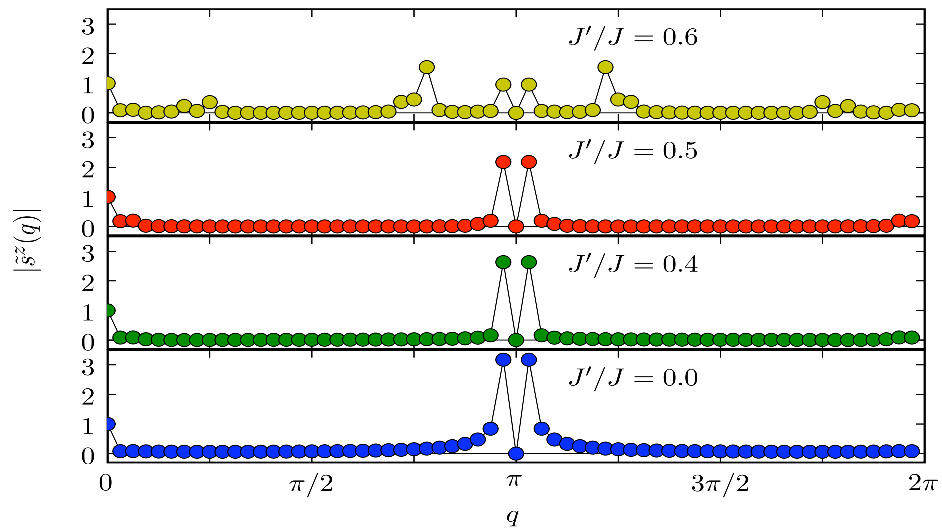
The momentum distribution $n(k)$
as a function of the parameter t' at $U = 3$.

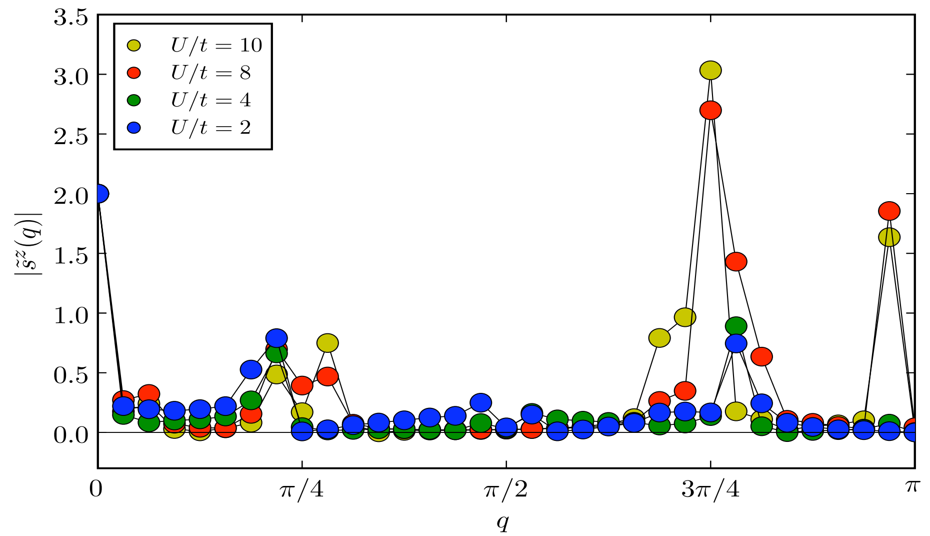
The Spin-Charge separation



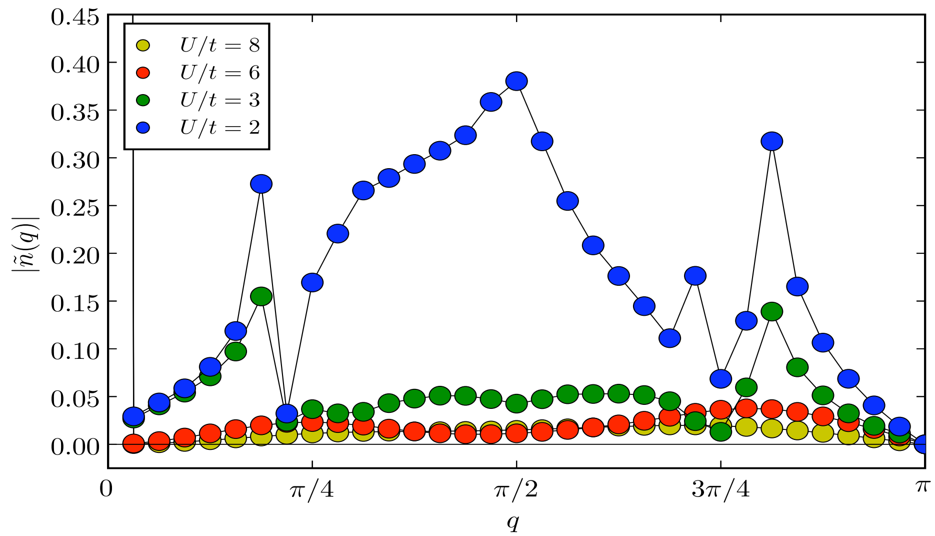


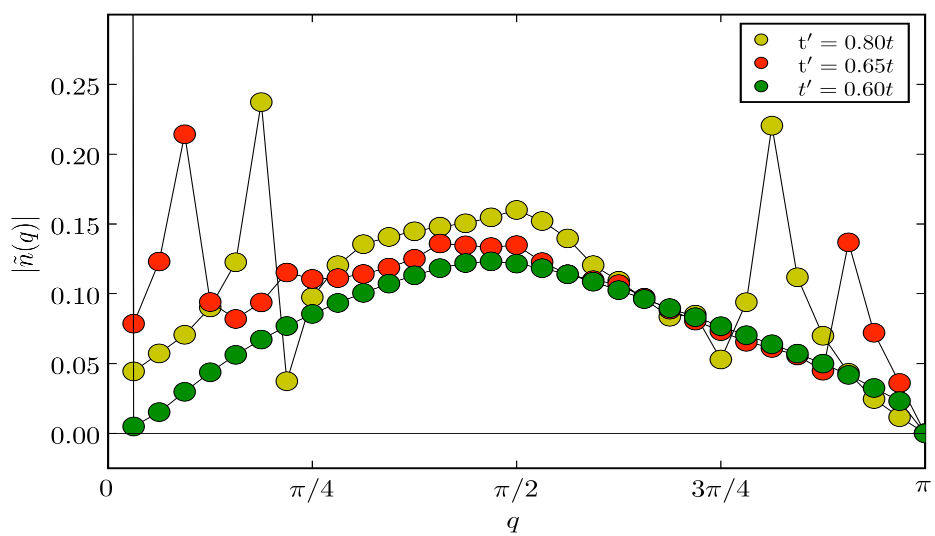
Spin distribution in the $S^z_{tot} = 1$ state



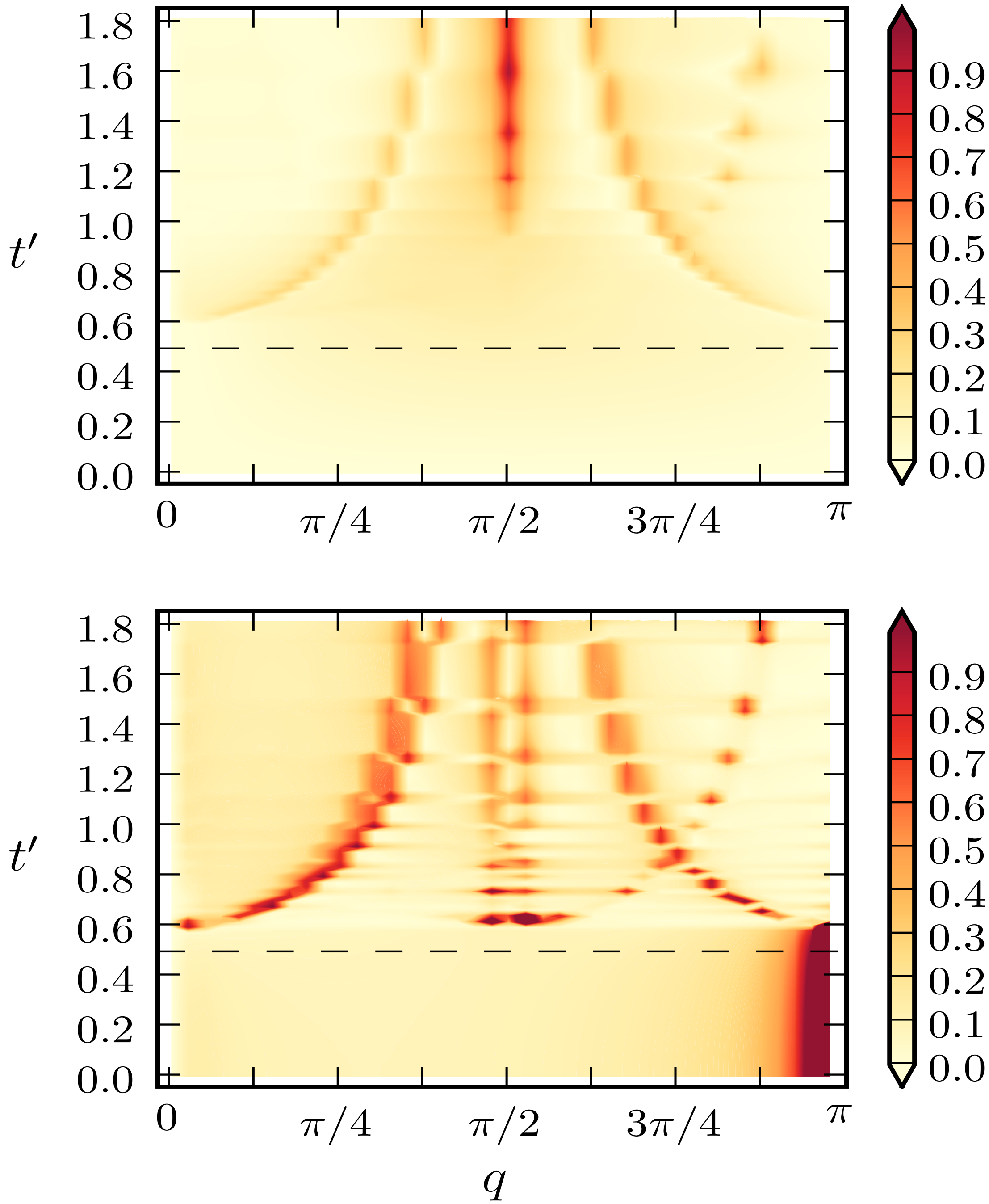


$S(q)$ **The Fourier transform of the Spin Distribution in the GS for** $t' = 3t$





$N(q)$ **the charge distribution in the ground state**



Fourier transform of the charge and spin distribution $|\langle N_q \rangle|$ and $|\langle S_q^z \rangle|$ as a function of t

Part II

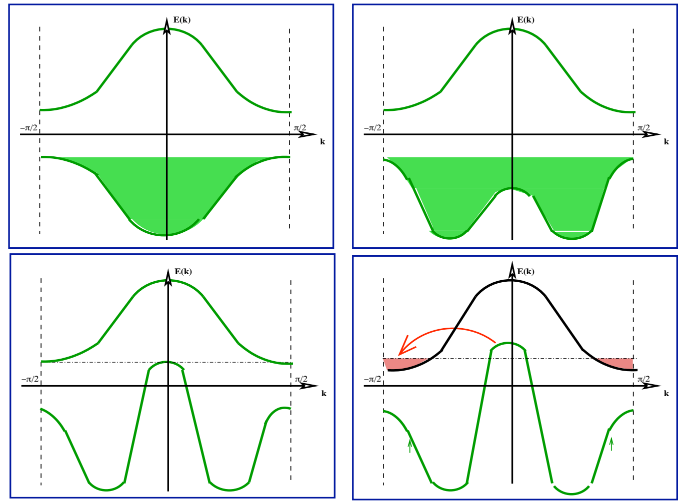
The ionic-Hubbard model

$$\mathcal{H} = -t \sum_{n,\sigma} \left(c^{\dagger}_{n,\sigma} c_{n+1,\sigma} + c^{\dagger}_{n+1,\sigma} c_{n,\sigma} \right)$$
$$+t' \sum_{n,\sigma} \left(c^{\dagger}_{n,\sigma} c_{n+2,\sigma} + c^{\dagger}_{n+2,\sigma} c_{n,\sigma} \right)$$
$$+\mu_0 \sum_{n,\sigma} \rho_{n,\sigma} + U \sum_{n} \rho_{n,\uparrow} \rho_{n,\downarrow}$$

The dispersion relation in the Free system: $U = 0$

$$E_{\pm}(k) = 2t' \cos 2k - \delta\mu \pm \sqrt{4t^2 \cos^2 k + (\Delta/2)^2} \, .$$

The Insulator to Metal transition in the free system!



At half-filling the excitation spectrum is gapped for

$$t' < t'_c = 0.5t\sqrt{1 + (\Delta/4t)^2} + \Delta/8$$

and gapless for $t' > t'_c$.

Bosonization

$$\mathcal{H} = \mathcal{H}_{\uparrow} + \mathcal{H}_{\downarrow}$$

$$\mathcal{H}_{\uparrow} = \int \mathbf{dx} \Big\{ \frac{\mathbf{v_F}}{\mathbf{2}} \big[(\partial_{\mathbf{x}} \mathbf{\Phi}_{\uparrow})^{\mathbf{2}} + (\partial_{\mathbf{x}} \mathbf{\Theta}_{\uparrow})^{\mathbf{2}} \big] - \frac{\mu_{eff}}{\sqrt{\pi}} \partial_x \Phi_{\uparrow} - \frac{\Delta}{2\pi a_0} \sin \sqrt{4\pi} \Phi_{\uparrow} \Big\}$$

$$\mathcal{H}_{\downarrow} = \int \mathbf{dx} \Big\{ \frac{\mathbf{v_F}}{\mathbf{2}} \big[(\partial_{\mathbf{x}} \mathbf{\Phi}_{\downarrow})^{\mathbf{2}} + (\partial_{\mathbf{x}} \mathbf{\Theta}_{\downarrow})^{\mathbf{2}} \big] - \frac{\mu_{\mathbf{eff}}}{\sqrt{\pi}} \partial_{\mathbf{x}} \mathbf{\Phi}_{\downarrow} - \frac{\mathbf{\Delta}}{\mathbf{2}\pi \mathbf{a_0}} \sin \sqrt{\mathbf{4}\pi} \mathbf{\Phi}_{\downarrow} \Big\},$$

where

$$\mu_{eff} = 2t' + \delta\mu = \begin{cases} 0 & \text{for} \quad t' < t'_* \\ 2\,(t' - t'_*) & \text{for} \quad t'_* < t' < t'_c \end{cases} .$$

and

$$t'_* = 0.5t\sqrt{1 + (\Delta/4t)^2} - \Delta/8$$

Sine-Gordon with $\beta = \sqrt{4\pi} \Leftrightarrow$ free Massive Thirring model

with the SOLITON MASS $= \Delta/2$

$$\mu_{eff} > \mu^c_{eff} = \Delta/2 \Rightarrow 2\,(t' - t'_*) = \Delta/2 \Rightarrow$$

$$t'_c = 0.5t\sqrt{1 + (\Delta/4t)^2} + \Delta/8$$

The ORDER Parameter for this transition is

$$\mathbf{N}_+ \sim q_0 \sim \sqrt{\mu - \mu_c}$$

Compressibility

$$\kappa = \partial E_0/\partial\mu \sim -k_0^{-1} = -(\mu - \mu_c)^{-1/2}\,,$$

The charge and spin field basis

Convenient basis for interacting electrons.

The Hamiltonian we have to consider now is given by

$$\begin{aligned}\mathcal{H} &= \int dx \Big\{ \frac{v_F}{2}\left[(\partial_x \varphi_c)^2 + (\partial_x \vartheta_c)^2\right] - \mu_{eff}\sqrt{\frac{2}{\pi}}\partial_x \varphi_c \\ &\quad + \frac{v_F}{2}\left[(\partial_x \varphi_s)^2 + \frac{1}{2}(\partial_x \vartheta_s)^2\right] \\ &\quad - \frac{\Delta}{\pi a_0}\sin\left(\sqrt{2\pi}\phi_c\right)\cos\left(\sqrt{2\pi}\phi_s\right)\Big\} .\end{aligned}$$

We decouple the interaction term in a mean-field manner by introducing

$$\begin{aligned} m_c &= \Delta \cdot \langle \cos(\sqrt{2\pi}\phi_s)\rangle \ , \\ m_s &= \Delta \cdot \langle \sin(\sqrt{2\pi}\phi_c)\rangle \ , \end{aligned}$$

The Mean-Field bosonized Hamiltonian

$$\mathcal{H}_c = \int dx \Big\{ \frac{v_F}{2}[P_c^2(x) + (\partial_x \phi_c)^2] - \mu_{eff}\sqrt{\frac{2}{\pi}}\partial_x \varphi_c - \frac{m_c}{\pi a_0}\sin(\sqrt{2\pi}\phi_c) \Big\},$$

$$\mathcal{H}_s = \int dx \Big\{ \frac{v_F}{2}[P_s^2(x) + (\partial_x \phi_s)^2] - \frac{m_s}{\pi a_0}\cos(\sqrt{2\pi}\phi_s) \Big\}.$$

$$M/\Lambda = \mathcal{C}_0\,(m/\Lambda)^{2/3}\;, \qquad \langle \cos\sqrt{2\pi}\varphi \rangle = \mathcal{C}_1\,(M/\Lambda)^{1/2}\;.$$

where

$$\mathcal{C}_0 = \frac{2\Gamma\,(1/6)}{\sqrt{\pi}\Gamma\,(2/3)}\left[\frac{\Gamma(3/4)}{2\Gamma(1/4)}\right]^{\frac{2}{3}}\;, \qquad \text{and} \qquad \mathcal{C}_1 = \frac{2}{3}\left(\frac{3\pi}{4}\right)^{1/4}\frac{\Gamma(3/4)}{\Gamma(1/4)}$$

and $\Lambda = 2t$ is the bandwidth.

Al. B. Zamolodchikov , Int. Jour. Mod. Phys. A **10**, 1125-1150 (1995).

S. Lukyanov, A. Zamolodchikov, Nucl.Phys. B **493**, 571 (1997).

$$
\begin{aligned}
M_c/\Lambda &= \mathcal{C}_0\,(\Delta/\Lambda)^{2/3}\,\langle\,\cos\sqrt{2\pi}\varphi_s\,\rangle^{2/3} \\
&= \mathcal{C}_0\,\mathcal{C}_1^{2/3}\,(\Delta/\Lambda)^{2/3}\,(M_s/\Lambda)^{1/3} \\
M_s/\Lambda &= \mathcal{C}_0\,(\Delta/\Lambda)^{2/3}\,\langle\,\sin\sqrt{2\pi}\varphi_c\,\rangle^{2/3} \\
&= \mathcal{C}_0\,\mathcal{C}_1^{2/3}\,(\Delta/\Lambda)^{2/3}\,(M_c/\Lambda)^{1/3}\ .
\end{aligned}
$$

The self-consistent solution gives

$$
M_c = M_s = \gamma\Delta/2
$$

where $\gamma = 2\mathcal{C}_0^{3/2}\mathcal{C}_1 = 1.74...$.

$$\mathcal{H}_c = \int dx \Big\{ \frac{v_F}{2}[P_c^2(x) + (\partial_x \phi_c)^2]$$
$$-\mu_{eff}\sqrt{\frac{2}{\pi}}\partial_x \varphi_c - \frac{m_c}{\pi a_0}\sin(\sqrt{2\pi}\phi_c)\Big\},$$

The SG field with $\beta^2 = 2\pi$: the excitation spectrum of the model consists of Solitons a antisolitons with mass M_c, and the soliton-antisoliton bound states ("breathers") with mas

$$M_c^{n=1} = 2M_c \sin(\pi/6) = M_c$$

and

$$M_c^{n=2} = 2M_c \sin(\pi/3) = \sqrt{3}M_c$$

.

The transition BI-METAL takes place when the effective chemical potential exceeds mass of the lowest breather i.e. at

$$\mu_{eff} > M_c = \Delta/2$$

.

The interacting case $U \neq 0$

$$\mathcal{H}_c = \int dx \Big\{ \frac{v_c}{2} \big[\frac{1}{K_c} (\partial_x \varphi_c)^2 + K_c (\partial_x \vartheta_c)^2 \big] - \mu_{eff} \sqrt{\frac{2}{\pi}} \partial_x \varphi_c$$
$$- \frac{m_c^r}{\pi a_0} \sin(\sqrt{2\pi} \phi_c) - \frac{M_c}{2\pi^2 a_0^2} \cos(2\sqrt{2\pi} \varphi_c) \Big\},$$
$$\mathcal{H}_s = \int dx \Big\{ \big[\frac{v_s}{2} (\partial_x \varphi_s)^2 + (\partial_x \vartheta_s)^2 \big] - \frac{m_s^r}{\pi a_0} \cos(\sqrt{2\pi} \phi_s) \Big\}.$$

where

$$m_c^r = \Delta_r \cdot \langle \cos(\sqrt{2\pi} \phi_s) \rangle \qquad m_s^r = \Delta_r \cdot \langle \sin(\sqrt{2\pi} \phi_c) \rangle \, ,$$

$M_c \sim U$ is the effective model parameters.

At $\mu_{eff} = 0$ the **Double sine-Gordon** model

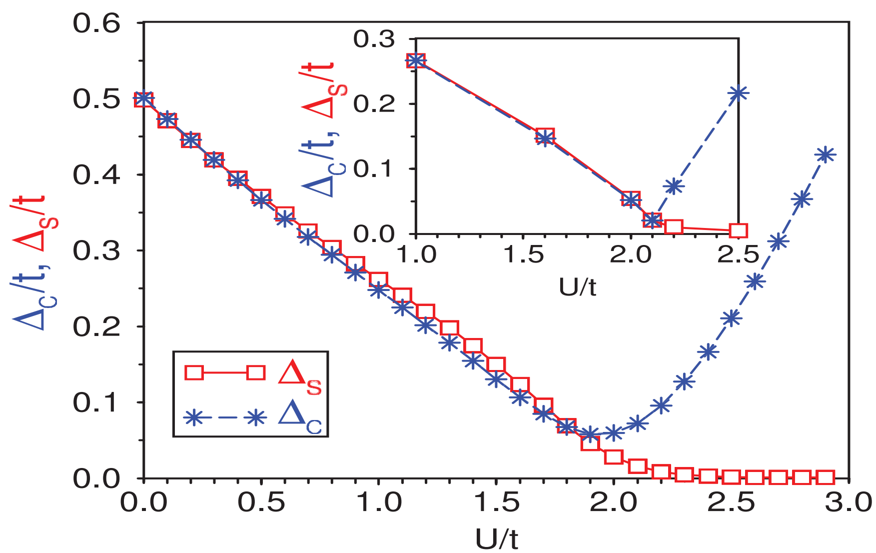
G. Delfino and G. Mussardo, Nucl.Phys. B 516, 675 (1998)

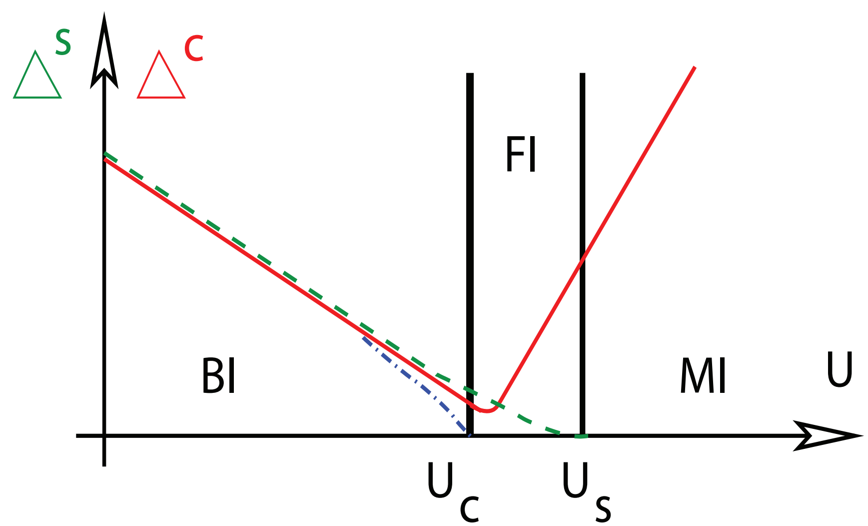
The Ionic-Hubbard model $(t' = \mu_{eff} = 0)$

M. Fabrizio, A. O. Gogolin, and A. A. Nersesyan, PRL **83**, 2014 (1999).

A. P. Kampf, M. Sekania, G. I. Japaridze, and P. Brune, J. Phys. C **15**, 5895 (2003).

S. R. Manmana, V. Meden, R. M. Noack, and K. Schönhammer, PRB **70**, 155115 (2004).





$$\mathcal{H}_c = \int dx \Big\{ \frac{v_c}{2}\big[(\partial_x \varphi_c)^2 + (\partial_x \vartheta_c)^2\big] - \mu_{\mathsf{eff}} \sqrt{\frac{2K_c}{\pi}} \partial_x \varphi_c$$
$$- \frac{m_c^r}{\pi a_0} \sin(\sqrt{2\pi K_c} \phi_c) \Big\},$$

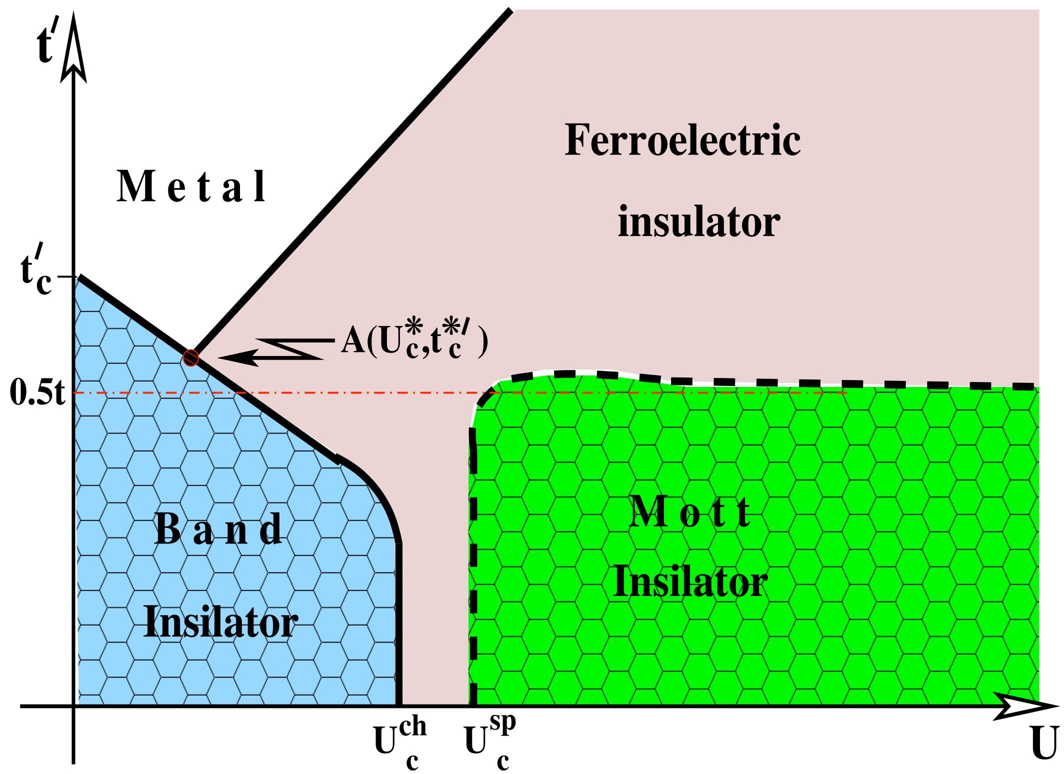
$$\mathcal{H}_c = \int dx \Big\{ \frac{v_c}{2}\big[(\partial_x \varphi_c)^2 + (\partial_x \vartheta_c)^2\big] - \mu_{\mathsf{eff}} \sqrt{\frac{2K_c}{\pi}} \partial_x \varphi_c$$
$$- \frac{M_c}{2\pi^2 a_0^2} \cos(2\sqrt{2\pi K_c} \varphi_c) \Big\},$$

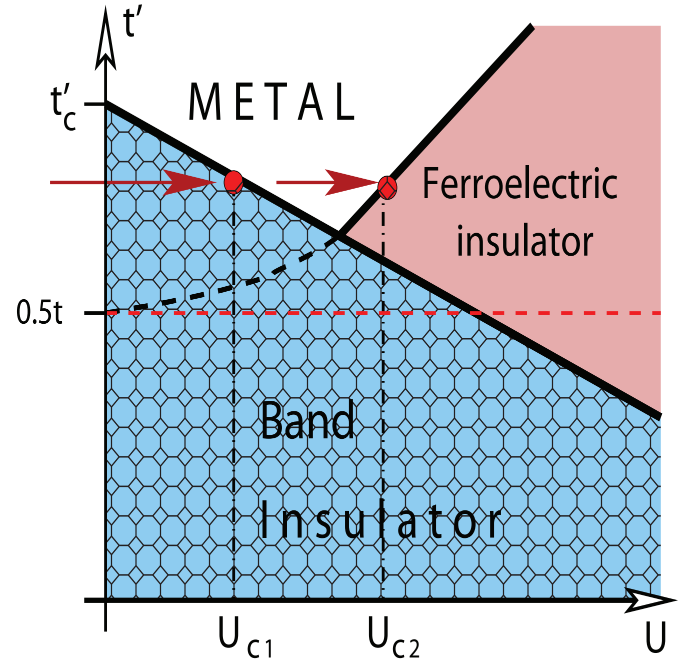
The band gap renormalizes with increasing U as

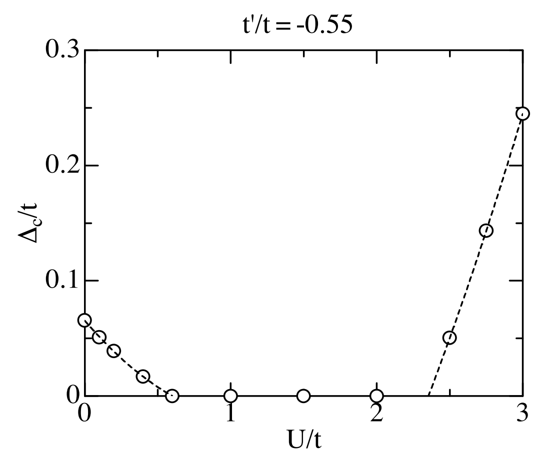
$$m_r = \Delta(1 - U/U^*)$$

Three different regimes:

- A. $\mu^r_{eff} < \Delta_r$. The Ionic-Hubbard sector
- B. $\mu_{eff} > \Delta_0$. The $t - t'$ Hubbard sector
- C. $\mu_{eff} > \Delta_0$. The new sector of phase diagram







Charge gap at $t' = 0.55t$ as a function of U.

The DMRG result by Satoshi Nishimoto

CONCLUSIONS

- We have shown that the gross features of the QFT from an insulator to a metal in the ground state of the $t - t'_c$ Hubbard model are well-described by the standard theory commensurate-incommensurate transitions

- We also obtain an analytical expression for the insulator-metal transition line $t'_c(U, t)$.

- Presented results of DMRG calculations of spin and charge distribution in various sect of the phase diagram which give evidence for the complete separation of the transiti involving spin and charge degrees of freedom.

- We have shown that in the GS of the $t - t'_c$ ionic-Hubbard model the Coulomb repuls driven transition Band-Insulator-Metall-Correlated (Mott) Insulator

- We have shown that the $t - t'_c$ ionic-Hubbard model could be a prototype model Ferroelectric Insulatores