Nonequilibrium quantum criticality of interacting Dirac fermions

Yin-Kai Yu (余荫铠)

yuyk6@mail2.sysu.edu.cn

www.yykspace.com

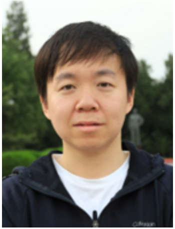
School of physics, Sun Yat-Sen University, Guangzhou 510275, China

第七届全国统计物理与复杂系统学术会议报告

2023 年 7 月 28 日

Collaborators

Zhi Zeng
(曾植)
SYSU



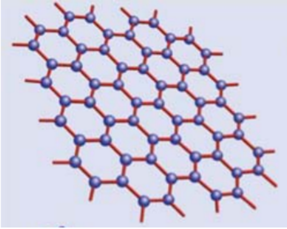
Zi-Xiang Li
(李自翔)
IOP, CAS

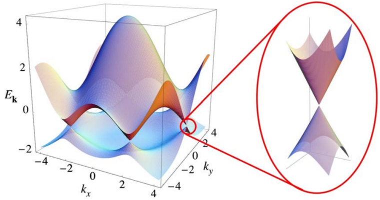
Shuai Yin
(阴帅)
SYSU

Contents

1. Background
2. Model and protocol
3. Imaginary-time relaxation dynamics with the AFM ordered initial state
4. Imaginary-time relaxation dynamics with the disordered initial state
5. Discussion and conclusion

Dirac fermion

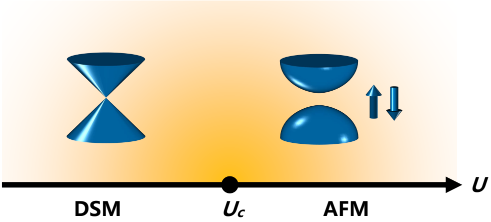




Dirac fermions, while being fundamentally significant in relativistic quantum field theories, are also prevalent as low-energy excitation quasi-particles in a diverse range of condensed-matter systems, including graphene, d-wave superconductors, Weyl/Dirac semimetals, and the surface of topological insulators.[1].

[1] Castro Neto, Guinea, Peres, Novoselov, and Geim, RMP, (2009).

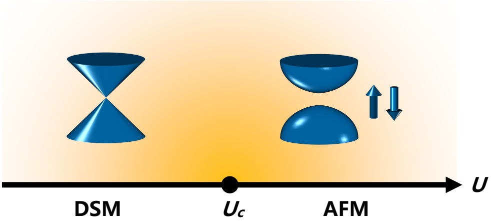
Interacting Dirac fermions



- The interactions between fermions cause a phase transition from Dirac semimetal to insulator.
- It's described by the **Gross-Neveu-Yukawa field theory**[2].
- Spontaneous symmetry breakings: $\mathbb{Z}_2$, $\mathrm{O}(2)$, $\mathrm{SU}(2)$.
- Due to the gapless fermionic fluctuations, universality classes: Wilson-Fisher $\Rightarrow$ chiral Ising, chiral XY and chiral Heisenberg.

[2] Gross and Neveu, PRD, (1974)
Wilson and Fisher, PRL, (1972)
Haldane, PRL, (1988).

Interacting Dirac fermions



- The interactions between fermions cause a phase transition from Dirac semimetal to insulator.
- It's described by the **Gross-Neveu-Yukawa field theory**[2].
- Spontaneous symmetry breakings: $\mathbb{Z}_2$, $\mathrm{O}(2)$, $\mathrm{SU}(2)$.
- Due to the gapless fermionic fluctuations, universality classes: Wilson-Fisher $\Rightarrow$ chiral Ising, chiral XY and chiral Heisenberg.

[2] Gross and Neveu, PRD, (1974)
Wilson and Fisher, PRL, (1972)
Haldane, PRL, (1988).

Nonequilibrium dynamics

For the critical phenomena, **nonequilibrium dynamics** is

- **fundamental: critical slowing down near the critical points.**
  — At the critical point, it takes an infinitely long time for the system to reach equilibrium. Therefore, what is actually observed as critical behavior is dynamic critical behavior.
- **useful: imaginary-time evolution recently finds its application in quantum computers.**[3]
  — Operating a quantum computer always involves non-equilibrium processes.

[3] Motta, Sun, Tan, ORourke, Ye, Minnich, Brandao, and Chan, Nat. Phys., (2020)
Nishi, Kosugi, and Matsushita, npj Quantum Inf., (2021).

Nonequilibrium dynamics

For the critical phenomena, **nonequilibrium dynamics** is

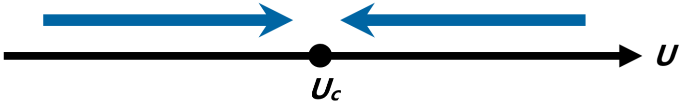
- **fundamental: critical slowing down near the critical points.**
  — At the critical point, it takes an infinitely long time for the system to reach equilibrium. Therefore, what is actually observed as critical behavior is dynamic critical behavior.
- **useful: imaginary-time evolution recently finds its application in quantum computers.**[3]
  — Operating a quantum computer always involves non-equilibrium processes.

[3] Motta, Sun, Tan, ORourke, Ye, Minnich, Brandao, and Chan, Nat. Phys., (2020)
Nishi, Kosugi, and Matsushita, npj Quantum Inf., (2021).

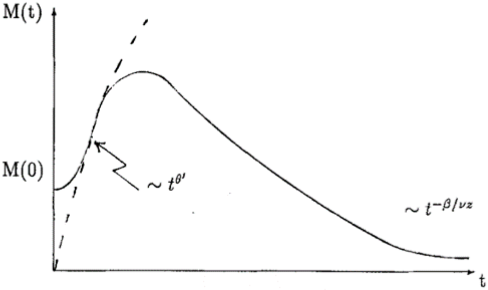
Relaxation

Relaxation is a most common approach to studying nonequilibrium dynamics.

1. Prepare a uncorrelated initial state.
2. Quench it to the critical point.
3. Explore the time evolution.



Relaxation in classical systems at the critical point



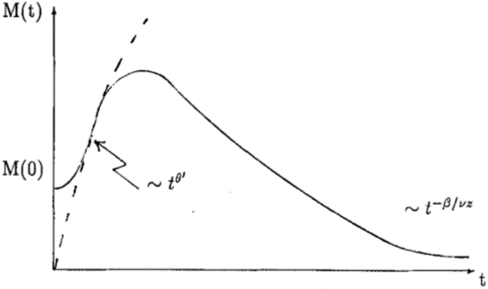
Relaxation in classical systems — real-time evolution

It is worth noting, **short time critical dynamics**[4]:

- **Critical initial slip** behavior — memory effects.
- Critical initial slip exponents θ.

[4] Janssen, Schaub, and Schmittmann, Z. Phys. B, (1989)
Li, Schülke, and Zheng, PRL, (1995)
Zheng, Int. J. Mod. Phys. B, (1998).

Relaxation in classical systems at the critical point

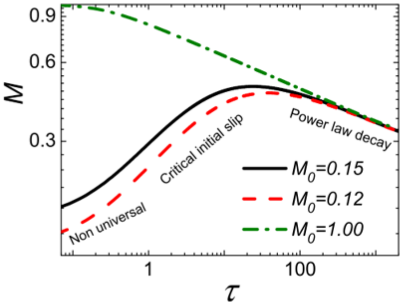


Relaxation in classical systems — real-time evolution
It is worth noting, **short time critical dynamics**[4]:

- **Critical initial slip** behavior — memory effects.
- Critical initial slip exponents θ.

[4] Janssen, Schaub, and Schmittmann, Z. Phys. B, (1989)
Li, Schülke, and Zheng, PRL, (1995)
Zheng, Int. J. Mod. Phys. B, (1998).

Relaxation in quantum systems at the critical point



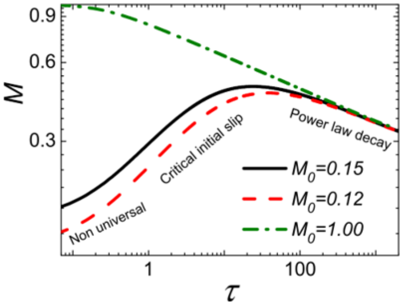
Relaxation in quantum systems — **imaginary-time evolution**

- amenability to large scale quantum Monte Carlo simulations
- is used to search for ground state in quantum computers[5]
- **short imaginary-time dynamics** at quanmtum critical point[6]

[5] Motta, Sun, Tan, ORourke, Ye, Minnich, Brandao, and Chan, Nat. Phys., (2020).

[6] Yin, Mai, and Zhong, PRL, (2014).

Relaxation in quantum systems at the critical point



Relaxation in quantum systems — **imaginary-time evolution**

- amenability to large scale quantum Monte Carlo simulations
- is used to search for ground state in quantum computers[5]
- **short imaginary-time dynamics** at quanmtum critical point[6]

[5] Motta, Sun, Tan, ORourke, Ye, Minnich, Brandao, and Chan, Nat. Phys., (2020).

[6] Yin, Mai, and Zhong, PRL, (2014).

Our motivation

Current status in this field:

- Quantum phase transitions in Dirac systems have attracted extensive attentions.
- The nonequilibrium dynamics has rarely been studied in fermionic systems.

Questions:

- What is the nonequilibrium dynamic behavior of interacting Dirac fermions near the critical point?
- How to determine the critical point and critical exponents of the Gross-Neveu-Yukawa universality classes using dynamical methods?
- How do gapless fermionic fluctuations affect short time scaling?

Our motivation

Current status in this field:

- Quantum phase transitions in Dirac systems have attracted extensive attentions.
- The nonequilibrium dynamics has rarely been studied in fermionic systems.

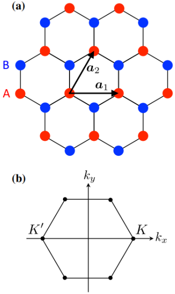
Questions:

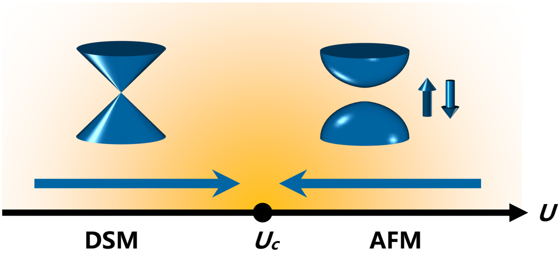
- What is the nonequilibrium dynamic behavior of interacting Dirac fermions near the critical point?
- How to determine the critical point and critical exponents of the Gross-Neveu-Yukawa universality classes using dynamical methods?
- How do gapless fermionic fluctuations affect short time scaling?

Contents

1. Background
2. Model and protocol
3. Imaginary-time relaxation dynamics with the AFM ordered initial state
4. Imaginary-time relaxation dynamics with the disordered initial state
5. Discussion and conclusion

Model





2D spin-$\frac{1}{2}$ Hubbard model on a half-filled honeycomb lattice[7]

$$H = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right). \tag{1}$$

[7] Boyack, Yerzhakov, and Maciejko, Eur. Phys. J. Spec. Top, (2021).

Model

Previous results in equilibrium research

model	**method**	U_c/t	ν	β
honeycomb	QMC[8]	3.85(2)	1.02(1)	0.76(2)
honeycomb	QMC[9]	3.77(4)	0.84(4)	0.71(8)
Gross-Neveu	$4-\epsilon$ (1st order)[10]	-	0.851	0.804
Gross-Neveu	$4-\epsilon$ (2nd order)[10]	-	1.01	0.995
Gross-Neveu	FRG[11]	-	1.31	1.31

Cannot reach a consensus within errorbar: U_c, ν.

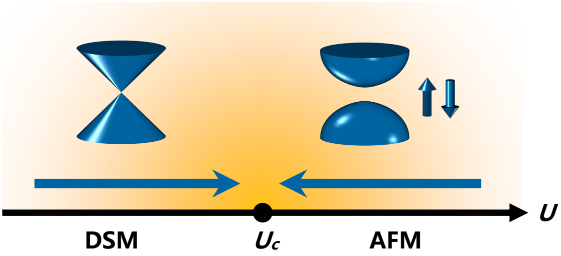
[8] Sorella, Otsuka, and Yunoki, PRX, (2016).

[9] Assaad, Parisen Toldin, Hohenadler, and Herbut, PRL, (2015).

[10] Rosenstein, Hoi-Lai Yu, and Kovner, Phys. Lett. B, (1993).

[11] Janssen and Herbut, PRL, (2014).

Protocol



Explore the imaginary-time relaxation near the critical point by determinant quantum Monte Carlo[12].

[12] Assaad, Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms, (2002).

Contents

1. Background
2. Model and protocol
3. Imaginary-time relaxation dynamics with the AFM ordered initial state
4. Imaginary-time relaxation dynamics with the disordered initial state
5. Discussion and conclusion

AFM order parameter m

AFM structure factor

$$S\left(\boldsymbol{q}\right)=\frac{1}{L^2}\sum_{i,j}\mathrm{e}^{\mathbf{i}\boldsymbol{q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}\langle m_i^{(z)}m_j^{(z)}\rangle, \tag{2}$$

where staggered magnetization $m_i^{(z)}$ is $m_i^{(z)}=\vec{c}_{i,A}^{\dagger}\sigma^z\vec{c}_{i,A}-\vec{c}_{i,B}^{\dagger}\sigma^z\vec{c}_{i,B}$. A and B represent different sublattices, $\vec{c}=(c_\uparrow,c_\downarrow)$.

AFM order parameter is

$$m^2=S\left(\mathbf{0}\right), \tag{3}$$

where $S\left(\mathbf{0}\right)$ is the AFM structure factor at zero momentum.

AFM order parameter m

AFM structure factor

$$S\left(\boldsymbol{q}\right)=\frac{1}{L^2}\sum_{i,j}\mathrm{e}^{\mathbf{i}\boldsymbol{q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}\langle m_i^{(z)}m_j^{(z)}\rangle, \tag{2}$$

where staggered magnetization $m_i^{(z)}$ is $m_i^{(z)}=\vec{c}_{i,A}^{\dagger}\sigma^z\vec{c}_{i,A}-\vec{c}_{i,B}^{\dagger}\sigma^z\vec{c}_{i,B}$. A and B represent different sublattices, $\vec{c}=(c_\uparrow,c_\downarrow)$.

AFM order parameter is

$$m^2=S\left(\mathbf{0}\right), \tag{3}$$

where $S\left(\mathbf{0}\right)$ is the AFM structure factor at zero momentum.

Determine the QCP

Dimensionless **correlation ratio**

$$R = S\left(\mathbf{0}\right)/S\left(\Delta \boldsymbol{q}\right), \tag{4}$$

where $\Delta \boldsymbol{q} = \left(\frac{1}{L}\boldsymbol{b}_1 + \frac{1}{L}\boldsymbol{b}_2\right)$ is minimum lattice momentum.

Saturated AFM initial state , near the equilibrium QCP universal scaling form

$$R\left(g, \tau, L\right) = f_R\left(gL^{1/\nu}, \tau L^{-z}\right), \tag{5}$$

where $g = \left(U - U_c\right)/t$, $z = 1$.

Determine the QCP

Dimensionless **correlation ratio**

$$R = S(\mathbf{0})/S(\Delta \boldsymbol{q}), \tag{4}$$

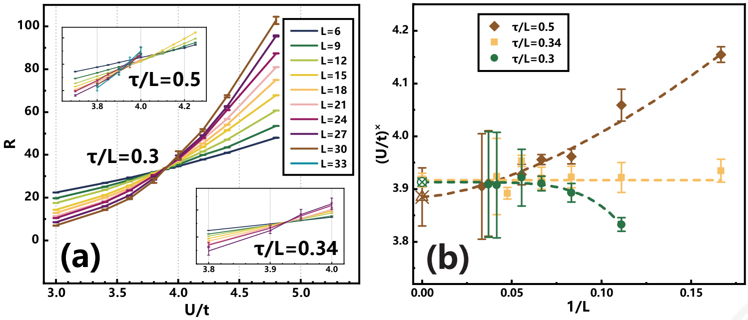
where $\Delta \boldsymbol{q} = \left(\frac{1}{L}\boldsymbol{b}_1 + \frac{1}{L}\boldsymbol{b}_2\right)$ is minimum lattice momentum.

Saturated AFM initial state , near the equilibrium QCP universal scaling form

$$R(g, \tau, L) = f_R\left(gL^{1/\nu}, \tau L^{-z}\right), \tag{5}$$

where $g = (U - U_c)/t$, $z = 1$.

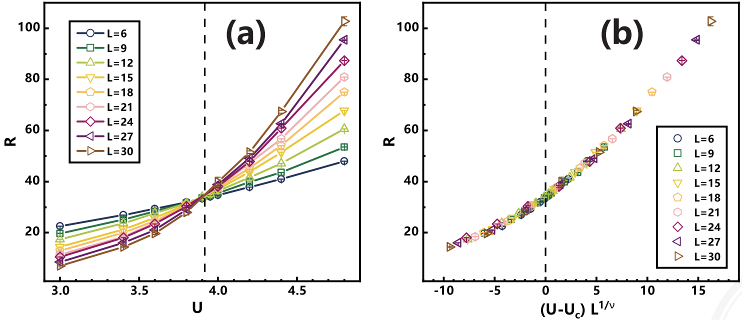
Estimation of quantum critical point U_c



$$R\left(g, \tau, L\right) = f_R\left(gL^{1/\nu}, \tau L^{-z}\right) \tag{6}$$

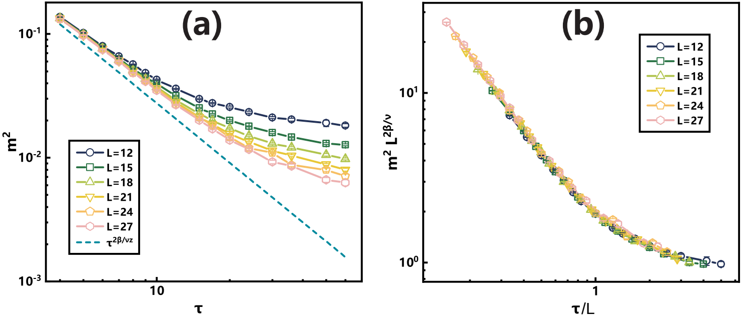
Fixed τL^{-z}, curves intersect at $g = U - U_c = 0$.
$\Rightarrow$ QCP: $U_c = 3.91 \pm 0.03 \quad (t = 1)$.

Fitting for ν



Fixing $\tau L^{-z} = 0.3,\ R(g) = f_R\left(gL^{1/\nu}\right)$,
$\Rightarrow\ \nu = 1.17 \pm 0.07$.

Fitting for β/ν



Saturated AFM initialized, $g = 0$ set,

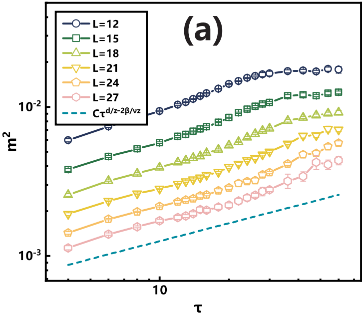
$$m^2 = \tau^{-2\beta/\nu z} f_{m^2}\left(\tau L^{-z}\right),$$

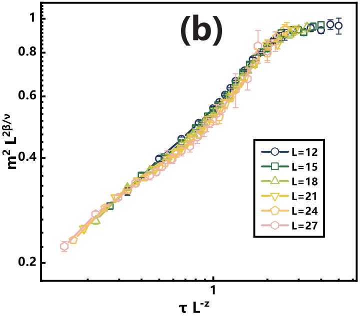
$\Rightarrow \ \beta/\nu = 0.80 \pm 0.03.$
Limit $\tau L^{-z} \to 0$, $m^2 \sim \tau^{-2\beta/\nu z} + \tau^{-2\beta/\nu z}\mathcal{O}(\tau L^{-z})$.

Contents

1. Background
2. Model and protocol
3. Imaginary-time relaxation dynamics with the AFM ordered initial state
4. Imaginary-time relaxation dynamics with the disordered initial state
5. Discussion and conclusion

Examination for β/ν





Initial DSM at $g = 0$. Here we take $\beta/\nu = 0.80$,

$$m^2 = L^{-d} \tau^{d/z - 2\beta/\nu z} f_{m^2}\left(\tau L^{-z}\right).$$

Compare with zero-order approximation $m^2 \sim \tau^{d/z - 2\beta/\nu z}$.

Fitting for θ

For the disordered initial state with random spins up or down, the **autocorrelation function** is defined as

$$A = \frac{1}{L^2} \overline{\sum_i \langle m_i^{(z)}(0)\, m_i^{(z)}(\tau) \rangle}. \tag{7}$$

where overline represents the average over various random initial states, and braket represents the expectation value in imaginary-time quantum mechanics.

Universal scaling at the critical point $g = 0$:

$$A = L^{\theta z - d} f_A\left(\tau^{-1} L^z\right). \tag{8}$$

Fitting for θ

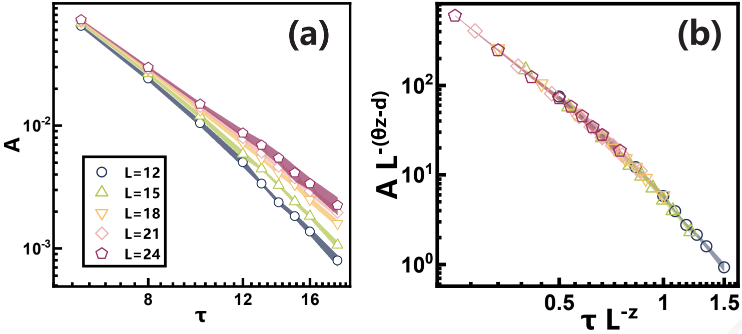
For the disordered initial state with random spins up or down, the **autocorrelation function** is defined as

$$A = \frac{1}{L^2} \overline{\sum_i \langle m_i^{(z)}(0)\, m_i^{(z)}(\tau) \rangle}. \tag{7}$$

where overline represents the average over various random initial states, and braket represents the expectation value in imaginary-time quantum mechanics.
Universal scaling at the critical point $g = 0$:

$$A = L^{\theta z - d} f_A \left(\tau^{-1} L^z \right). \tag{8}$$

Fitting for θ



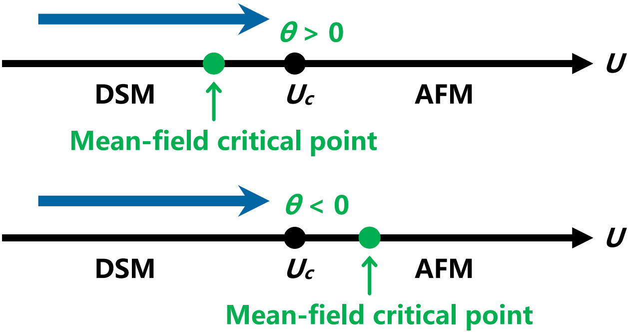
Random initial state at $g = 0$,

$$A = L^{\theta z - d} f_A \left(\tau^{-1} L^z \right).$$

$\Rightarrow \ \theta = -0.84 \pm 0.04.$

Negative θ

Critical initial slip exponent θ is negative.



Contents

1. Background
2. Model and protocol
3. Imaginary-time relaxation dynamics with the AFM ordered initial state
4. Imaginary-time relaxation dynamics with the disordered initial state
5. Discussion and conclusion

Discussion

model	**method**	U_c/t	β/ν	θ
honeycomb	QMC (present)	3.91(3)	0.80(3)	$-0.84(4)$
honeycomb	QMC[13]	3.85(2)	0.75(2)	-
honeycomb	QMC[14]	3.77(4)	0.8(1)	-
Gross-Neveu	$4-\epsilon$ (1st order)[15]	-	0.945	-
Gross-Neveu	$4-\epsilon$ (2nd order)[15]	-	0.985	-
Gross-Neveu	FRG[16]	-	1.008	-

Controversial ν: present $1.17(7)$, Sorella $1.02(1)$ and Assaad$0.84(4)$.

[13] Sorella, Otsuka, and Yunoki, PRX, (2016).

[14] Assaad, Parisen Toldin, Hohenadler, and Herbut, PRL, (2015).

[15] Rosenstein, Hoi-Lai Yu, and Kovner, Phys. Lett. B, (1993).

[16] Janssen and Herbut, PRL, (2014).

Conclusion

- For the first time, we demonstrate the nonequilibrium dynamics of interacting Dirac fermions.
- We develop a dynamical methods to determine the critical point and critical exponents of the chiral Heisenberg universality class.
- Specifically, we obtain $U_c = 3.91(3)$ and $\nu = 1.17(7) > 1$ using the dynamic method.
- We find a negative critical initial slip exponent $\theta = -0.84(4)$.

Thanks for your attention!

Conclusion

- For the first time, we demonstrate the nonequilibrium dynamics of interacting Dirac fermions.
- We develop a dynamical methods to determine the critical point and critical exponents of the chiral Heisenberg universality class.
- Specifically, we obtain $U_c = 3.91(3)$ and $\nu = 1.17(7) > 1$ using the dynamic method.
- We find a negative critical initial slip exponent $\theta = -0.84(4)$.

Thanks for your attention!

Conclusion

- For the first time, we demonstrate the nonequilibrium dynamics of interacting Dirac fermions.
- We develop a dynamical methods to determine the critical point and critical exponents of the chiral Heisenberg universality class.
- Specifically, we obtain $U_c = 3.91(3)$ and $\nu = 1.17(7) > 1$ using the dynamic method.
- We find a negative critical initial slip exponent $\theta = -0.84(4)$.

Thanks for your attention!

Conclusion

- For the first time, we demonstrate the nonequilibrium dynamics of interacting Dirac fermions.
- We develop a dynamical methods to determine the critical point and critical exponents of the chiral Heisenberg universality class.
- Specifically, we obtain $U_c = 3.91(3)$ and $\nu = 1.17(7) > 1$ using the dynamic method.
- We find a negative critical initial slip exponent $\theta = -0.84(4)$.

Thanks for your attention!

Conclusion

- For the first time, we demonstrate the nonequilibrium dynamics of interacting Dirac fermions.
- We develop a dynamical methods to determine the critical point and critical exponents of the chiral Heisenberg universality class.
- Specifically, we obtain $U_c = 3.91(3)$ and $\nu = 1.17(7) > 1$ using the dynamic method.
- We find a negative critical initial slip exponent $\theta = -0.84(4)$.

Thanks for your attention!