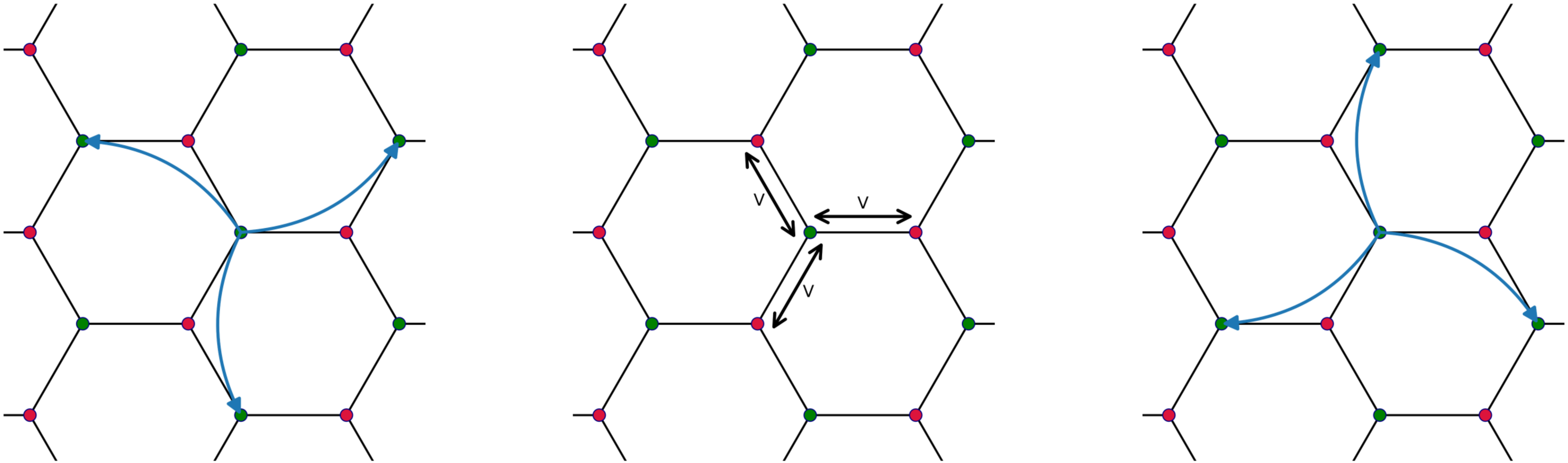


HYBRID MONTE CARLO FOR THE EXTENDED KANE-MELE-HUBBARD MODEL

JULY 30TH 2026 I FINN TEMMEN I FORSCHUNGSZENTRUM JÜLICH

HYBRID MONTE CARLO FOR THE EXTENDED KANE-MELE-HUBBARD MODEL

JULY 30TH 2026 I FINN TEMMEN I FORSCHUNGSZENTRUM JÜLICH

IN COLLABORATION WITH

THOMAS LUU (FORSCHUNGSZENTRUM JÜLICH)

JOHANN OSTMEYER (UNIVERSITY OF BONN)

LIN WANG (FORSCHUNGSZENTRUM JÜLICH)

MOTIVATION

Hubbard model

$a_x, a_x^\dagger \ldots$ spin-$\uparrow$ particle

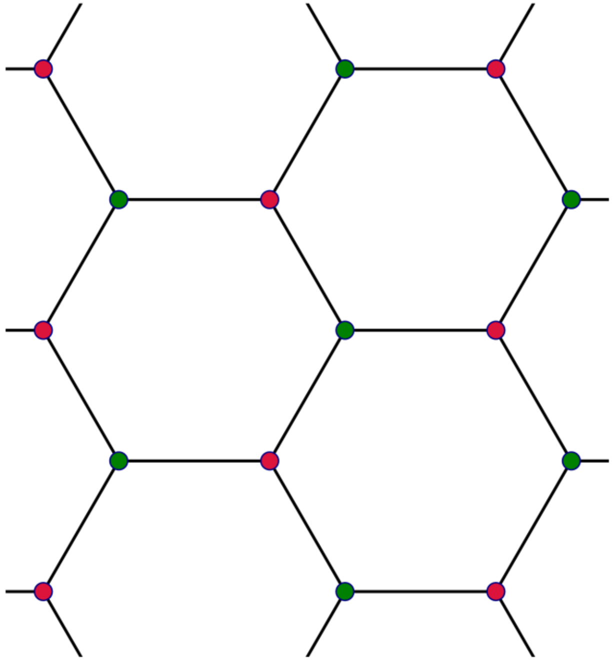
$b_x, b_x^\dagger \ldots$ spin-$\downarrow$ hole

$q_x = a_x^\dagger a_x$

$\tilde{q}_x = b_x^\dagger b_x$

$$H_{\text{Hub}} = -t \sum_{\langle x,y \rangle} \left(a_x^\dagger a_y - b_x^\dagger b_y + \text{h.c.} \right) - U \sum_x q_x \tilde{q}_x + \mu \sum_x (q_x - \tilde{q}_x)$$

- Simulations of **Graphene**



MOTIVATION

Hubbard model

$a_x, a_x^\dagger \ldots$ spin- $\uparrow$ particle

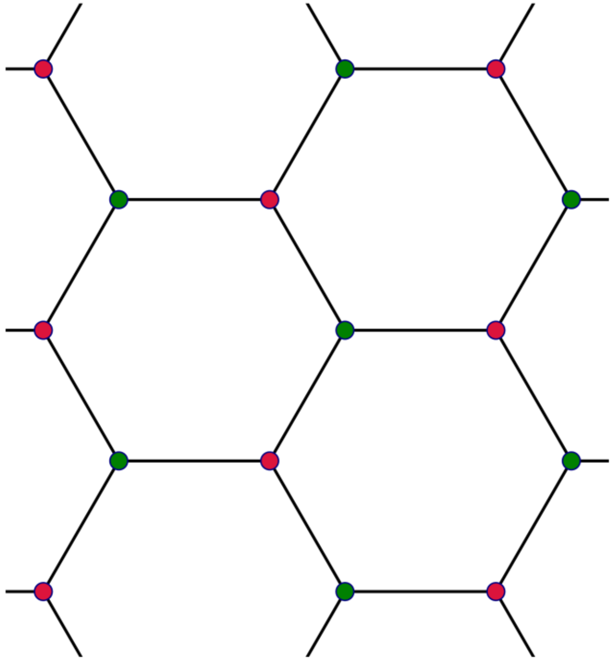
$b_x, b_x^\dagger \ldots$ spin- $\downarrow$ hole

$q_x = a_x^\dagger a_x$

$\tilde{q}_x = b_x^\dagger b_x$

$$H_{\mathrm{Hub}} = -t \sum_{\langle x,y \rangle} \left(a_x^\dagger a_y - b_x^\dagger b_y + \mathrm{h.c.} \right) - U \sum_x q_x \tilde{q}_x + \mu \sum_x (q_x - \tilde{q}_x)$$

- Simulations of **Graphene**
- **Hubbard model** on **honeycomb lattice** $(N_x = 2L^2)$
  - Nearest-neighbor hopping t
  - On-site interaction U
  - Chemical potential μ (half-filling at $\mu = 0$)



JÜLICH Forschungszentrum

MOTIVATION

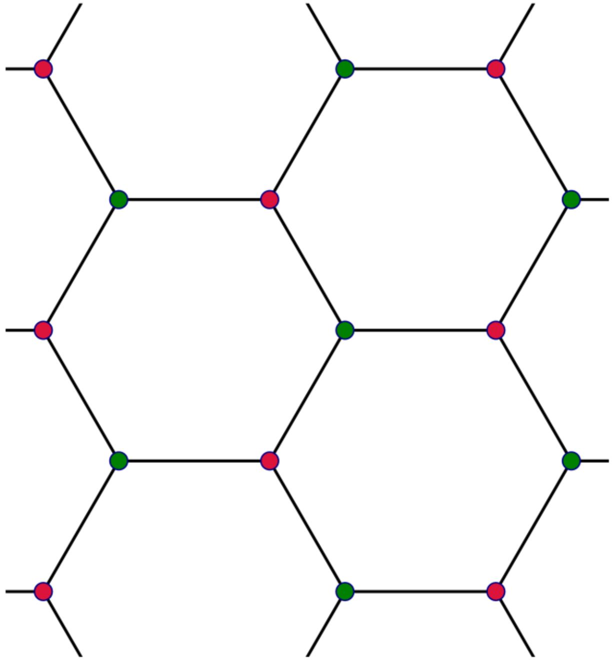
Hubbard model

$a_x, a_x^\dagger \ldots$ spin-$\uparrow$ particle
$b_x, b_x^\dagger \ldots$ spin-$\downarrow$ hole
$q_x = a_x^\dagger a_x$
$\tilde{q}_x = b_x^\dagger b_x$

$$H_{\text{Hub}} = -t \sum_{\langle x,y \rangle} \left(a_x^\dagger a_y - b_x^\dagger b_y + \text{h.c.}\right) - U \sum_x q_x \tilde{q}_x + \mu \sum_x (q_x - \tilde{q}_x)$$

- Simulations of **Graphene**
- **Hubbard model** on **honeycomb lattice** $(N_x = 2L^2)$
    - Nearest-neighbor hopping t
    - On-site interaction U
    - Chemical potential μ (half-filling at $\mu = 0$)

- Powerful **minimal description** but room for improvement!



JÜLICH Forschungszentrum

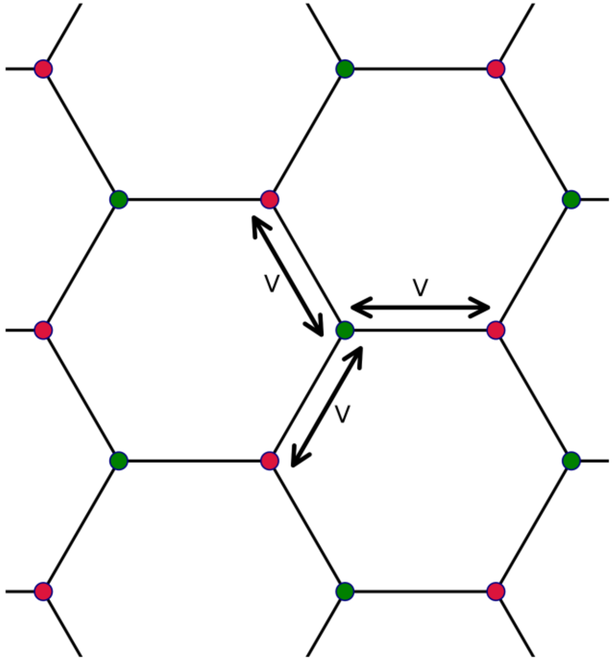
EXTENDED HUBBARD MODEL

Getting closer to reality

$a_x, a_x^\dagger \ldots \text{spin-} \uparrow \text{ particle}$
$b_x, b_x^\dagger \ldots \text{spin-} \downarrow \text{ hole}$
$q_x = a_x^\dagger a_x$
$\tilde{q}_x = b_x^\dagger b_x$

$$H_{\text{eHub}} = H_{\text{Hub}} + V \sum_{\langle x,y \rangle} (q_x - \tilde{q}_x)(q_y - \tilde{q}_y)$$

- Non-local interactions
  - Coulomb-Hubbard model: Coulomb potential
  - Pariser-Parr-Pople (PPP) model: Ohno/Mataga-Nishimoto potential
  - **Extended Hubbard model**: nearest-neighbor interaction V



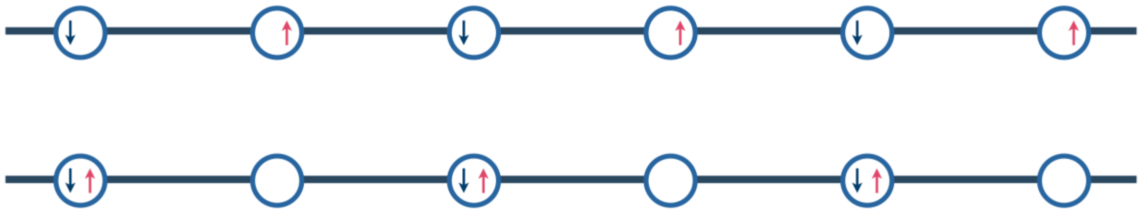
EXTENDED HUBBARD MODEL

Getting closer to reality

$a_x, a_x^\dagger \ldots$ spin-$\uparrow$ particle
$b_x, b_x^\dagger \ldots$ spin-$\downarrow$ hole
$q_x = a_x^\dagger a_x$
$\tilde{q}_x = b_x^\dagger b_x$

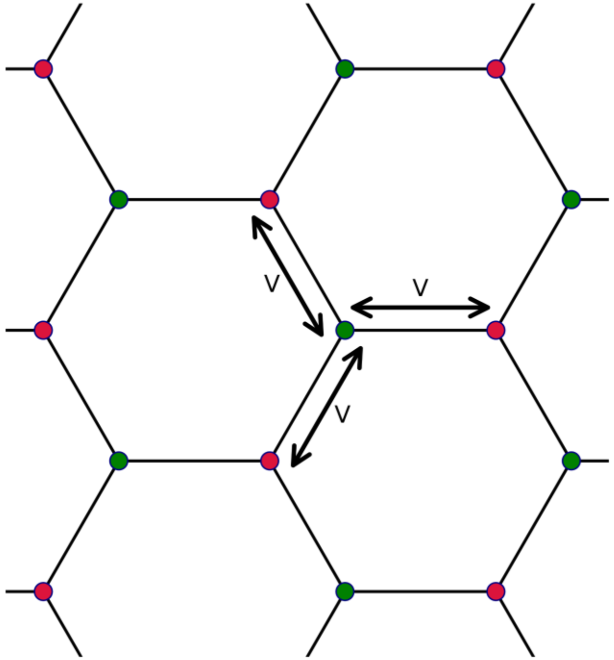
$$H_{\text{eHub}} = H_{\text{Hub}} + V \sum_{\langle x,y \rangle} (q_x - \tilde{q}_x)(q_y - \tilde{q}_y)$$

- Non-local interactions
  - Coulomb-Hubbard model: Coulomb potential
  - Pariser-Parr-Pople (PPP) model: Ohno/Mataga-Nishimoto potential
  - **Extended Hubbard model**: nearest-neighbor interaction V
- Competition of U and V
  - **Spin density wave** (SDW/AFM) vs **charge density wave** (CDW)



SDW

CDW



JÜLICH Forschungszentrum

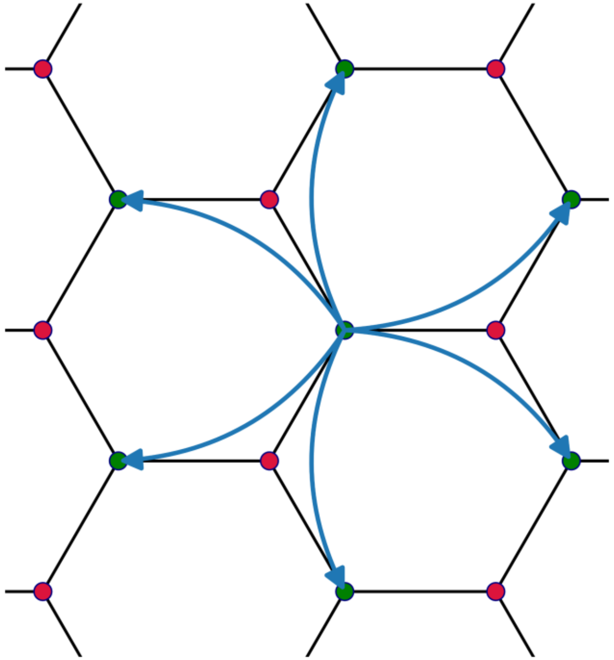
EXTENDED KANE-MELE-HUBBARD MODEL

Getting closer to reality

$a_x, a_x^\dagger \ldots$ spin- $\uparrow$ particle
$b_x, b_x^\dagger \ldots$ spin- $\downarrow$ hole
$q_x = a_x^\dagger a_x$
$\tilde{q}_x = b_x^\dagger b_x$

$$H_{\text{eKMH}} = H_{\text{eHub}} + i\lambda_{\text{SO}} \sum_{\langle\langle x,y \rangle\rangle} \nu_{xy} \left(a_x^\dagger a_y - b_x^\dagger b_y\right)$$

- Spin-orbit coupling (λ_{SO}) term
  - Charged particle moving in potential experiences magnetic field
  - Particle's spin gives intrinsic magnetic moment
  - Effective magnetic field couples to spin magnetic moment



- **Kane-Mele model**
  - (counter-)Clockwise hopping: $\nu_{xy} = \pm 1$
- **Quantum spin Hall insulator**

Kane, Mele, PRL **95** (2005)

JÜLICH Forschungszentrum

EXTENDED KANE-MELE-HUBBARD MODEL

Getting closer to reality

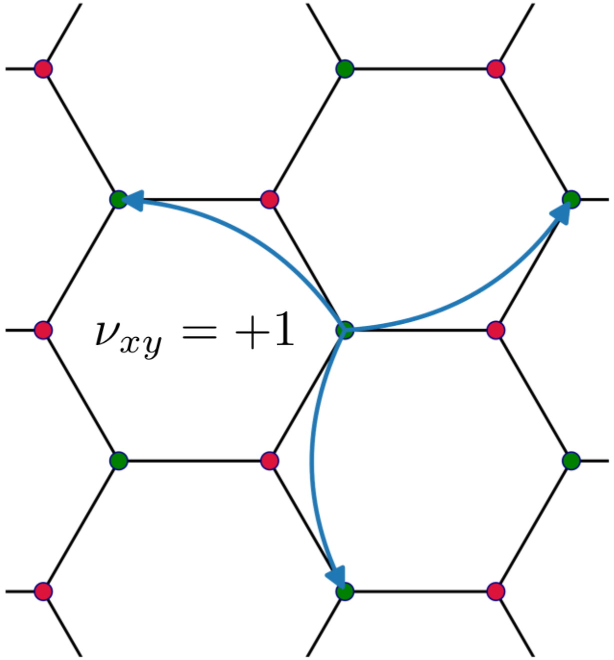
$a_x, a_x^\dagger \ldots \text{spin-} \uparrow \text{ particle}$
$b_x, b_x^\dagger \ldots \text{spin-} \downarrow \text{ hole}$
$q_x = a_x^\dagger a_x$
$\tilde{q}_x = b_x^\dagger b_x$

$$H_{\text{eKMH}} = H_{\text{eHub}} + i\lambda_{\text{SO}} \sum_{\langle\langle x,y \rangle\rangle} \nu_{xy} \left(a_x^\dagger a_y - b_x^\dagger b_y \right)$$

- Spin-orbit coupling (λ_{SO}) term
  - Charged particle moving in potential experiences magnetic field
  - Particle's spin gives intrinsic magnetic moment
  - Effective magnetic field couples to spin magnetic moment

- **Kane-Mele model**
  - (counter-)Clockwise hopping: $\nu_{xy} = \pm 1$
- **Quantum spin Hall insulator**

Kane, Mele, PRL **95** (2005)



JÜLICH Forschungszentrum

EXTENDED KANE-MELE-HUBBARD MODEL

Getting closer to reality

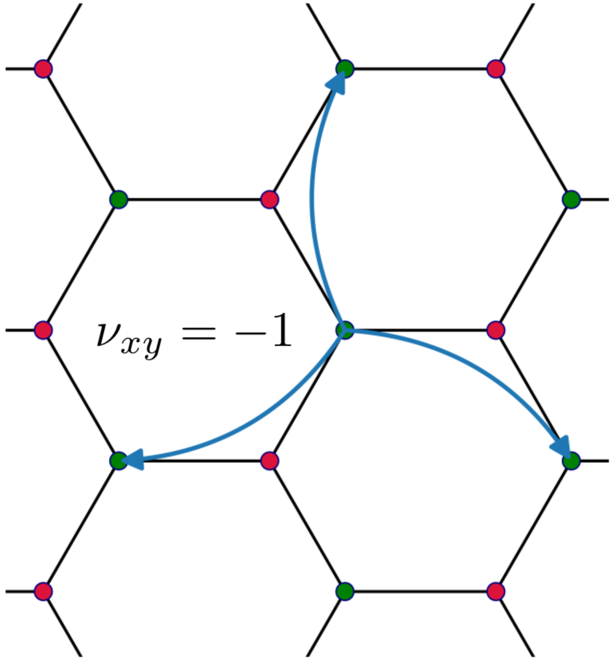
$a_x, a_x^\dagger \ldots$ spin-$\uparrow$ particle
$b_x, b_x^\dagger \ldots$ spin-$\downarrow$ hole
$q_x = a_x^\dagger a_x$
$\tilde{q}_x = b_x^\dagger b_x$

$$H_{\text{eKMH}} = H_{\text{eHub}} + i\lambda_{\text{SO}} \sum_{\langle\langle x,y \rangle\rangle} \nu_{xy} \left(a_x^\dagger a_y - b_x^\dagger b_y \right)$$

- Spin-orbit coupling (λ_{SO}) term
    - Charged particle moving in potential experiences magnetic field
    - Particle's spin gives intrinsic magnetic moment
    - Effective magnetic field couples to spin magnetic moment

Kane, Mele, PRL **95** (2005)

- **Kane-Mele model**
    - (counter-)Clockwise hopping: $\nu_{xy} = \pm 1$
- **Quantum spin Hall insulator**



PATH INTEGRAL FORMALISM

Decoupling many-body interactions

- Decouple many-body interactions with **Hubbard-Stratonovich (HS) transformation**

$$\exp\left\{\pm\frac{|\alpha|}{2}\mathcal{O}^2\right\} = \frac{1}{\mathcal{N}}\int d\phi\,\exp\left\{-\frac{\phi^2}{2|\alpha|} - \sqrt{\pm 1}\,\phi\mathcal{O}\right\}$$

PATH INTEGRAL FORMALISM

Decoupling many-body interactions

- Decouple many-body interactions with **Hubbard-Stratonovich (HS) transformation**

$$\exp\left\{\pm\frac{|\alpha|}{2}\mathcal{O}^2\right\} = \frac{1}{\mathcal{N}}\int d\phi\,\exp\left\{-\frac{\phi^2}{2|\alpha|} - \sqrt{\pm 1}\,\phi\mathcal{O}\right\}$$

- **Complete the squares** for U and V

$$Q_x = q_x - \tilde{q}_x$$

$$V\sum_{\langle x,y\rangle} Q_x Q_y = \frac{V}{2}\sum_{\langle x,y\rangle}\left(Q_x + Q_y\right)^2 + 3V\sum_x q_x\tilde{q}_x \;+\; \text{bilinear}$$

$$-(U-3V)\sum_x q_x\tilde{q}_x = \frac{1}{2}(U-3V)\sum_x Q_x^2 \;+\; \text{bilinear}$$

PATH INTEGRAL FORMALISM

Decoupling many-body interactions

$$Q_x = q_x - \tilde{q}_x$$

- HS transformation depends on $\boldsymbol{U}$ **vs** $\boldsymbol{V}$

$$\exp\left\{-\Delta_t (U - 3V) Q_x^2\right\} \propto \int d\phi_{tx} \exp\left\{-\frac{\phi^2}{2\Delta_t |U - 3V|} - \sqrt{-\operatorname{sgn}(U - 3V)}\,\phi_{tx} Q_x\right\}$$

JÜLICH Forschungszentrum

PATH INTEGRAL FORMALISM

Decoupling many-body interactions

$$Q_x = q_x - \tilde{q}_x$$

- HS transformation depends on $\boldsymbol{U}$ **vs** $\boldsymbol{V}$

$$\exp\left\{-\Delta_t (U-3V) Q_x^2\right\} \propto \int d\phi_{tx} \exp\left\{-\frac{\phi^2}{2\Delta_t |U-3V|} - \sqrt{-\mathrm{sgn}\,(U-3V)}\phi_{tx} Q_x\right\}$$

- **Sign problem free** at half-filling for $U \geq 3V$ **(golden region)** Zheng et al. PRB **84** (2011)

$$S[\phi,\chi] = \sum_{t,x} \frac{\phi_{tx}^2}{2\Delta_t |U-KV|} + \sum_{t,\langle x,y\rangle} \frac{\chi_{txy}^2}{2\Delta_t V} - \log\det M[i\phi, i\chi] - \log\det \bar{M}[i\phi, i\chi]$$

JÜLICH Forschungszentrum

PATH INTEGRAL FORMALISM

Decoupling many-body interactions

$$Q_x = q_x - \tilde{q}_x$$

- HS transformation depends on $\boldsymbol{U}$ **vs** $\boldsymbol{V}$

$$\exp\left\{-\Delta_t (U-3V) Q_x^2\right\} \propto \int d\phi_{tx} \exp\left\{-\frac{\phi^2}{2\Delta_t |U-3V|} - \sqrt{-\mathrm{sgn}\,(U-3V)}\,\phi_{tx} Q_x\right\}$$

- **Sign problem free** at half-filling for $U \geq 3V$ **(golden region)** Zheng et al. PRB **84** (2011)

$$S[\phi,\chi] = \sum_{t,x} \frac{\phi_{tx}^2}{2\Delta_t |U-KV|} + \sum_{t,\langle x,y\rangle} \frac{\chi_{txy}^2}{2\Delta_t V} - \log\det M[i\phi, i\chi] - \log\det \bar{M}[i\phi, i\chi]$$

- **Prohibitive (?) sign problem** for $3V > U$ **(forbidden region)**

$$S[\phi,\chi] = \sum_{t,x} \frac{\phi_{tx}^2}{2\Delta_t |U-KV|} + \sum_{t,\langle x,y\rangle} \frac{\chi_{txy}^2}{2\Delta_t V} - \log\det M[\phi, i\chi] - \log\det \bar{M}[\phi, i\chi]$$

ALGORITHM

- **Hybrid Monte Carlo** (HMC)

  Duane et al. PLB **195** (1987)

ALGORITHM

- **Hybrid Monte Carlo** (HMC)

  Duane et al. PLB **195** (1987)

Kennedy, Yu PoS Lattice (2024)
Ostmeyer JPA **58** (2025)
FT et al. PRB **112** (2025)

- **Radial updates**
  - Improve convergence properties
  - Ergodicity in presence of infinite potential barriers

$$
\begin{aligned}
&\textbf{Sample}\quad \gamma \sim \mathcal{N}(0,\sigma^2);\\
&\textbf{Propose}\quad \phi' \leftarrow \phi_{\text{init}} e^{\gamma};\\
&\textbf{Compute}\quad \Delta S \leftarrow S(\phi') - S(\phi_i);\\
&\textbf{accept/reject}\ \text{with}\ e^{-\Delta S + d\gamma};
\end{aligned}
$$

ALGORITHM

- **Hybrid Monte Carlo** (HMC)

  Duane et al. PLB **195** (1987)

Kennedy, Yu PoS Lattice (2024)
Ostmeyer JPA **58** (2025)
FT et al. PRB **112** (2025)

- **Radial updates**
  - Improve convergence properties
  - Ergodicity in presence of infinite potential barriers

$$
\begin{aligned}
&\textbf{Sample} \quad \gamma \sim \mathcal{N}(0, \sigma^2);\\
&\textbf{Propose} \quad \phi' \leftarrow \phi_{\text{init}} e^{\gamma};\\
&\textbf{Compute} \quad \Delta S \leftarrow S(\phi') - S(\phi_i);\\
&\textbf{accept/reject} \text{ with } e^{-\Delta S + d\gamma};
\end{aligned}
$$

Luu, FT et al. arXiv:2604.00815 (2026)

- **Stabilization**
  - Numerical instabilities with increasing β
  - Amplified in extended Hubbard model
  - Separation of scales with QR decompositions

JÜLICH Forschungszentrum

QUANTIFYING THE SIGN PROBLEM

Transition from golden to forbidden region

- **Average phase**

$$\Sigma = |\langle e^{-i\mathrm{Im}(S)}\rangle_{\mathrm{Re}(S)}|$$

- **Effective sample size**

$$N_{\mathrm{eff}} \propto \Sigma^2 N$$

QUANTIFYING THE SIGN PROBLEM

Transition from golden to forbidden region

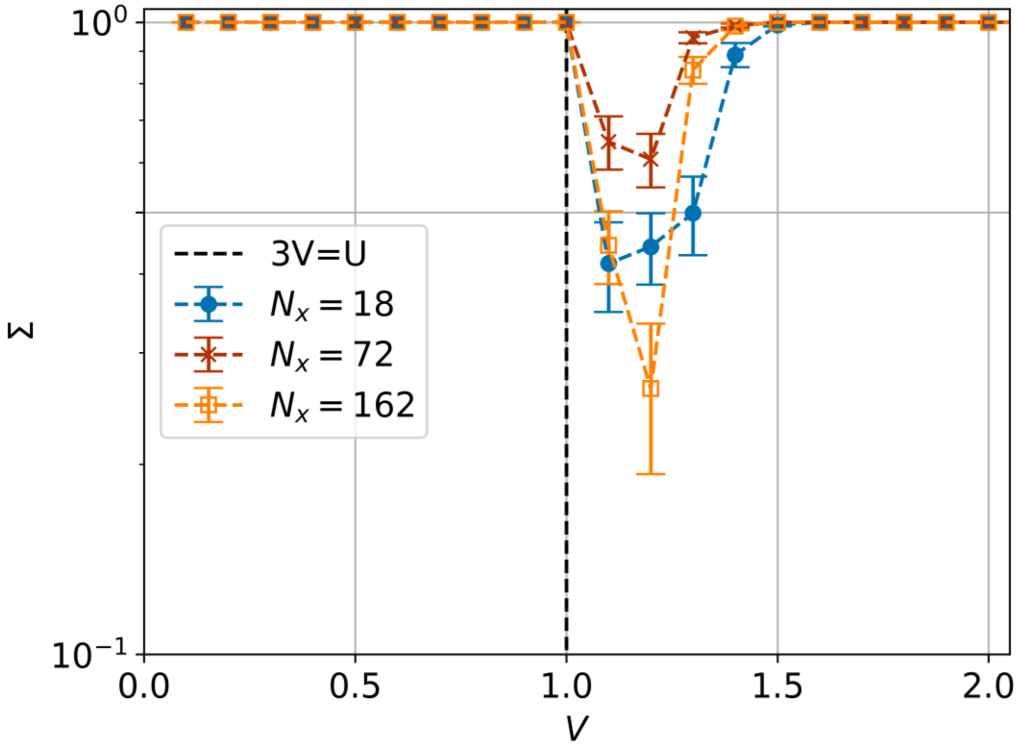
$U = 3$
$\beta = 4$
$\mu = \text{half-filling}$
$\lambda_{\text{SO}} = 0$

- **Average phase**

$$\Sigma = |\langle e^{-i\text{Im}(S)}\rangle_{\text{Re}(S)}|$$

- **Effective sample size**

$$N_{\text{eff}} \propto \Sigma^2 N$$



JÜLICH Forschungszentrum

QUANTIFYING THE SIGN PROBLEM

Transition from golden to forbidden region

$U = 3$
$\beta = 4$
$\mu = \text{half-filling}$
$\lambda_{\text{SO}} = 0$

- **Average phase**

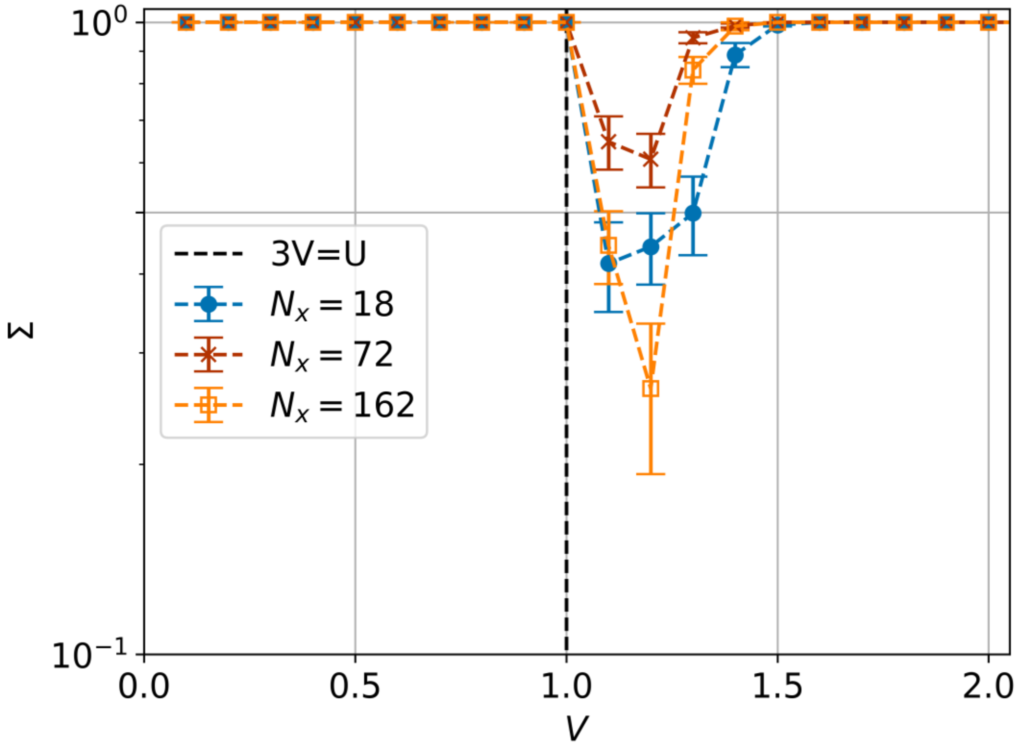
$$\Sigma = |\langle e^{-i\text{Im}(S)} \rangle_{\text{Re}(S)}|$$

- **Effective sample size**

$$N_{\text{eff}} \propto \Sigma^2 N$$

- Leverage bad Σ to locate phase transition

Mondaini et al. PRB **107** (2023)
Kennedy et al. PRB **111** (2025)



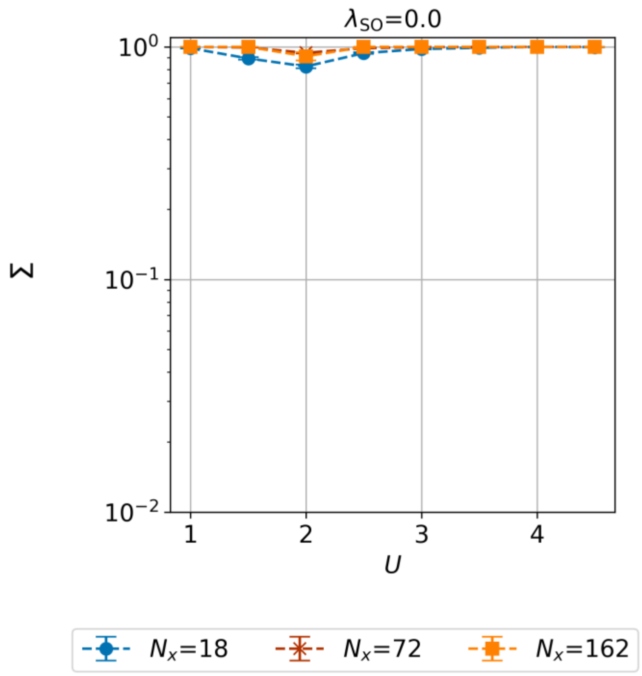
QUANTIFYING THE SIGN PROBLEM

Forbidden region $(3V \geq U)$

$3V/U = 1.5$

$\beta = 4$

$\mu = \text{half-filling}$

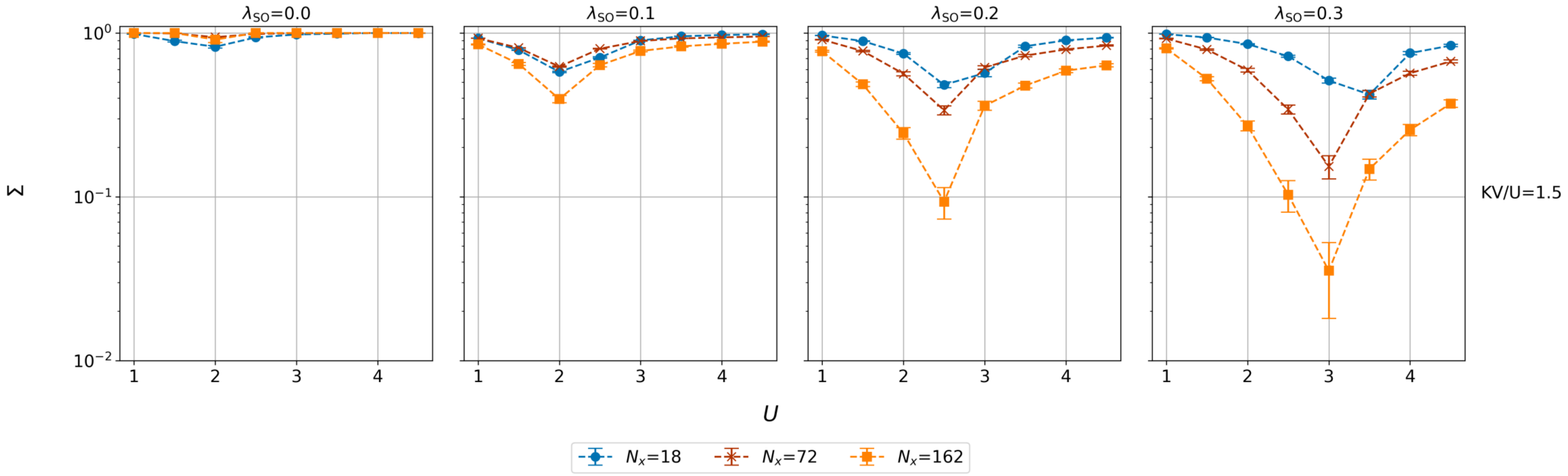


JÜLICH Forschungszentrum

QUANTIFYING THE SIGN PROBLEM

Forbidden region $(3V \geq U)$

$3V/U = 1.5$
$\beta = 4$
$\mu = \text{half-filling}$

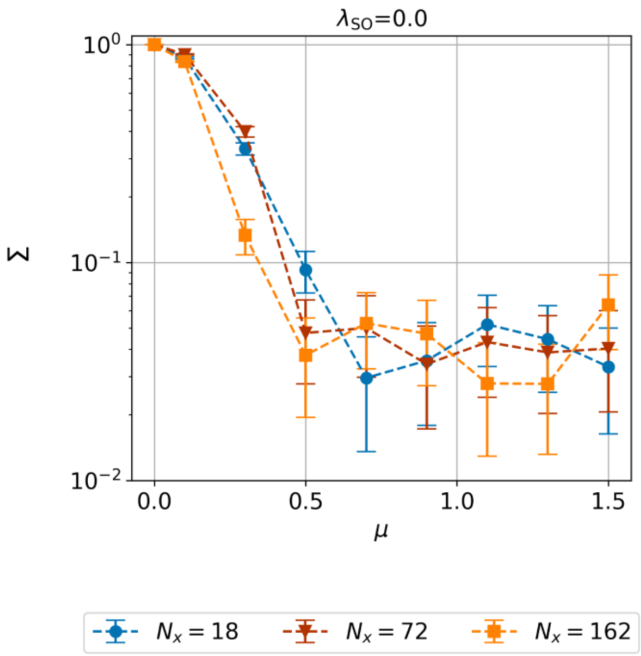


JÜLICH Forschungszentrum

QUANTIFYING THE SIGN PROBLEM

All that glitters is not gold $(3V < U)$

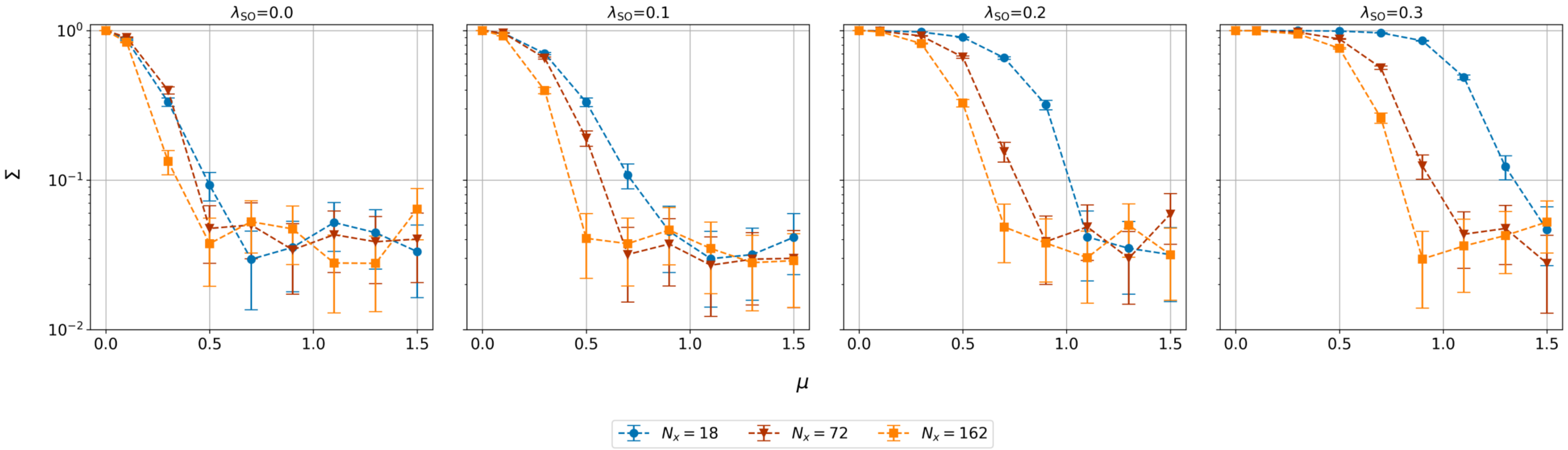
$U = 2$
$3V/U = 0.9$
$\beta = 4$



QUANTIFYING THE SIGN PROBLEM

All that glitters is not gold $(3V < U)$

$U = 2$
$3V/U = 0.9$
$\beta = 4$



SUMMARY AND OUTLOOK

- Formalism for **HMC** simulations of the **Extended Kane-Mele-Hubbard model**
    - **Sign problem free** simulations only in **golden region** $3V \leq U$
    - **Unavoidable sign** problem in **forbidden region** $3V > U$

SUMMARY AND OUTLOOK

- Formalism for **HMC** simulations of the **Extended Kane-Mele-Hubbard model**
    - **Sign problem free** simulations only in **golden region** $3V \leq U$
    - **Unavoidable sign** problem in **forbidden region** $3V > U$

- **Map out phase diagram:**
    - Forbidden region $\boldsymbol{U, V, \lambda_{SO}}$
    - Extend system sizes up to $L = 18$ ($N_x = 648$)
    - Approaching prohibitive sign problem from below and above in V
    - Golden region $\boldsymbol{\mu, \lambda_{SO}}$
    - Revisit half-filled golden region at large β with numerical stabilization

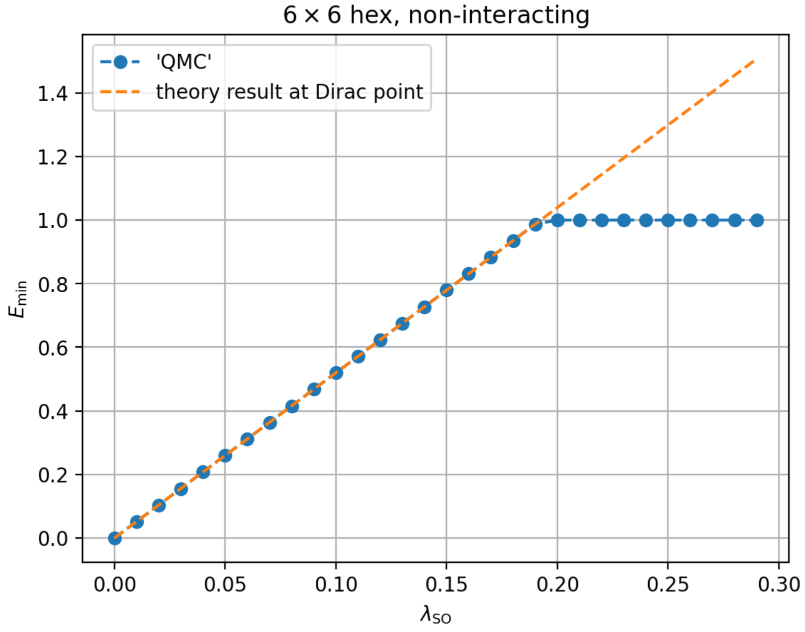
BACKUP SLIDES

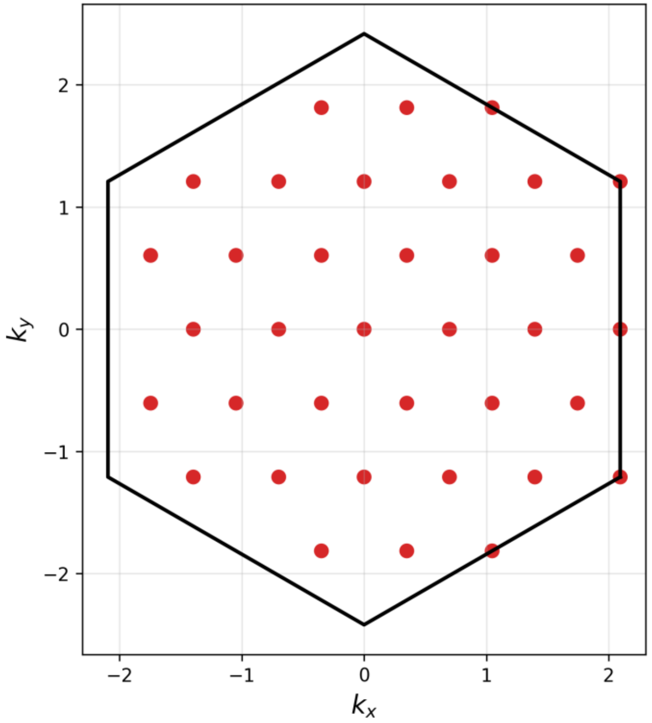
GROUND STATE

Turning on spin orbit coupling

- Spin orbit coupling increases K point energy overtaking M point

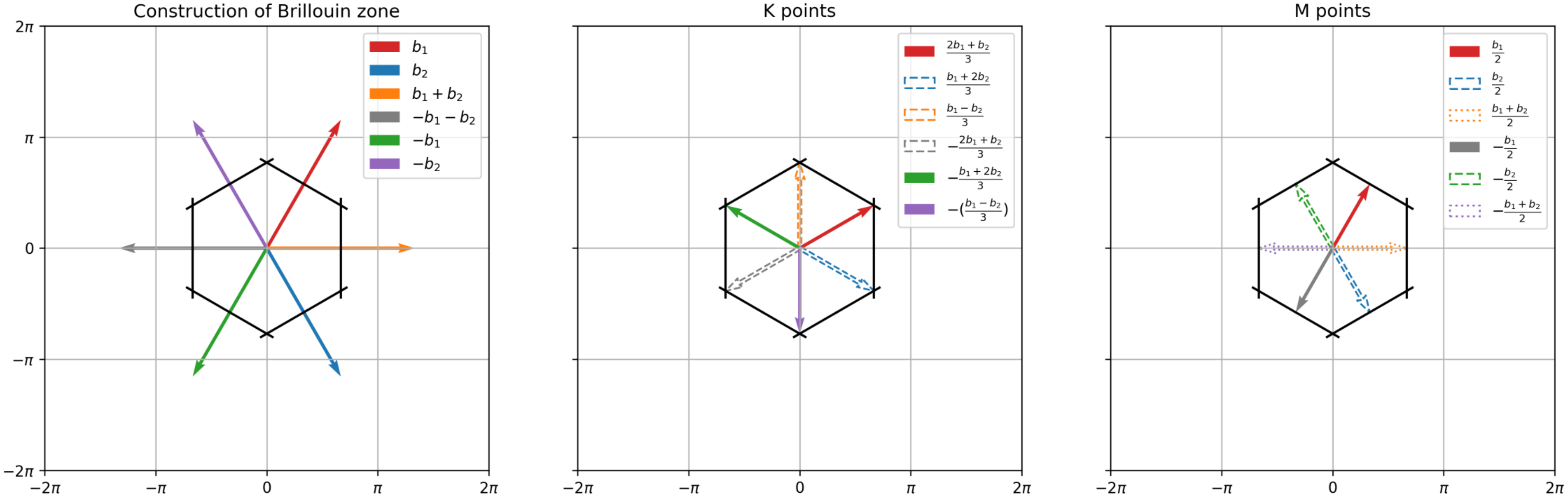
$$E_K = 3\sqrt{3}\lambda_{SO}$$





BRILLOUIN ZONE

Construction and K, M points



ORDER PARAMETERS

- Spin density wave: **Staggered spin structure factor**

$$S_{\text{SDW}} = \frac{1}{N_x^2}\langle S_-^z S_-^z \rangle_c \quad \text{with} \quad S_-^z = \frac{1}{2}\sum_x (S_{Ax}^z - S_{Bx}^z) \quad \text{and} \quad S_i^z = c_{\uparrow i}^\dagger c_{\uparrow i} - c_{\downarrow i}^\dagger c_{\downarrow i}$$

- Charge density wave: **Staggered density structure factor**

$$S_{\text{CDW}} = \frac{1}{N_x^2}\langle Q_- Q_- \rangle_c \quad \text{with} \quad Q_- = \sum_x (n_{Ax} - n_{Bx}) \quad \text{and} \quad n_i = n_{\uparrow i} + n_{\downarrow i}$$

- Quantum spin hall insulator: **no local order parameter**
  - Z_2 topological invariant
  - Bulk gap with no SDW/CDW