

Entanglement Hamiltonian and spectra from quantum Monte Carlo simulations of interacting fermions.

Fakher F. Assaad (KITP, June 23rd 2015)

Organization

- Introduction: Entanglement Hamiltonian and spectra for free electrons.
- QMC
 - Weak coupling approaches → Gaussian representation of reduced density matrix
 - Strong coupling approaches → Replica
- Conclusions



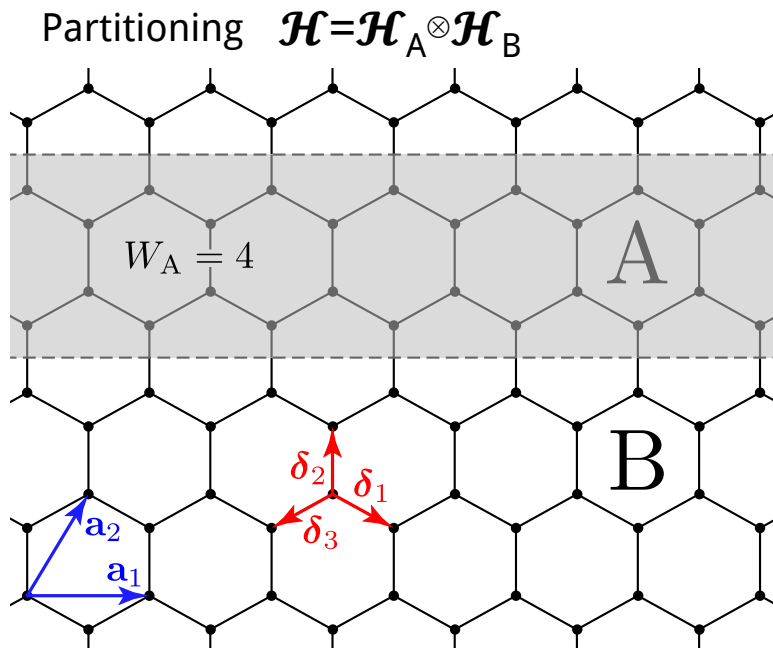
F. Parisen Toldin



T. Lang

Discussions with Tarun Grover

Entanglement Hamiltonian for non-interacting systems



$$\hat{\rho}_A = \text{Tr}_B \hat{\rho} = e^{-\hat{H}_E}, \quad \hat{\rho} = \frac{e^{-\beta \hat{H}_0}}{Z}$$

$$\hat{\rho}_A = \det [1 - G_A] e^{-\hat{\mathbf{a}}^\dagger \ln [G_A^{-1} - 1] \hat{\mathbf{a}}}$$

G_A Single particle equal time Green function matrix in \mathcal{H}_A

$\forall \hat{O} \in \mathcal{H}_A$ Wick's theorem leads to

$$\text{Tr}_A \hat{\rho}_A \hat{O} = \text{Tr} \hat{\rho} \hat{O} \quad \text{since}$$

$$\text{Tr}_A [\hat{\rho}_A \hat{a}_x \hat{a}_y^\dagger] \stackrel{!}{=} \text{Tr} [\hat{\rho} \hat{a}_x \hat{a}_y^\dagger] = [G_A]_{xy}$$

$$\frac{1}{2} - G_A = \frac{1}{2} \tanh(H_E / 2)$$

Insulating states. Band flattening.

$\frac{1}{2} - G$ and H_0 are adiabatically connected
 \rightarrow Have the same topological properties

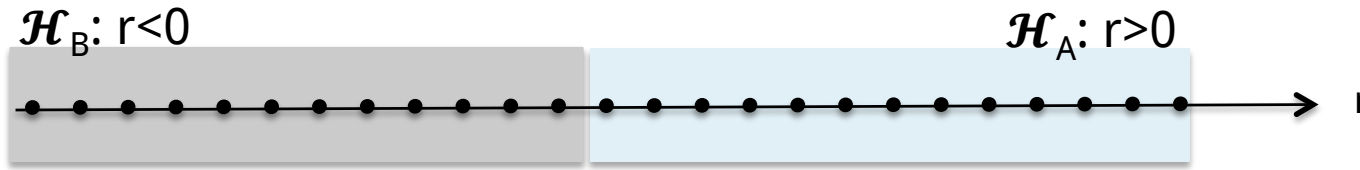
I. Peschel, Journal of Physics A 36, L205 (2003)

L. Fidkowski. Phys. Rev. Lett., 104, 130502, (2010)

A. M. Turner, Y. Zhang, and A. Vishwanath
 Phys. Rev. B, 82, 241102, (2010)

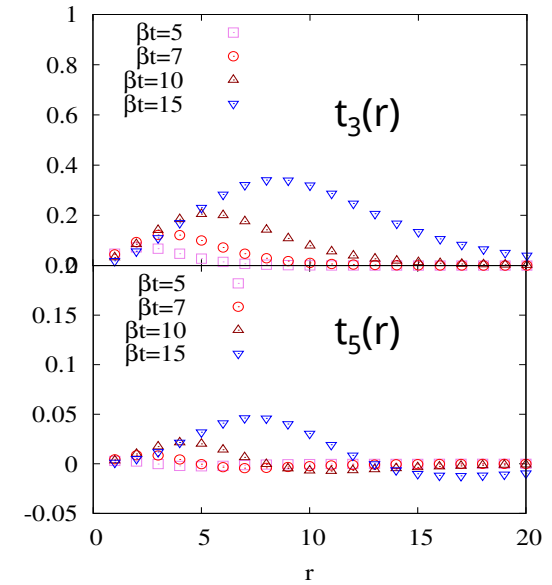
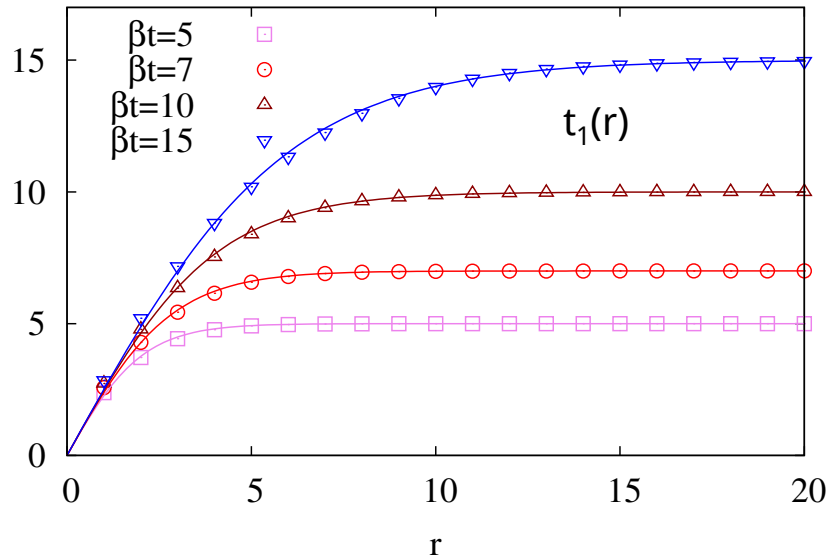
Entanglement Hamiltonian of a tight binding chain

Partitioning $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ $H_0 = t \sum_i (\hat{c}_i^\dagger \hat{c}_{i+1} + h.c.)$



$$H_E = \sum_{n,r>0} t_n(r) (\hat{c}_r^\dagger \hat{c}_{r+n} + h.c.) \cong \sum_{r>0} t \beta \tanh\left(\frac{\alpha}{\beta} r\right) (\hat{c}_r^\dagger \hat{c}_{r+1} + h.c.), \quad \alpha \cong 2.5 / t$$

$$L = 256, L_A = 128$$

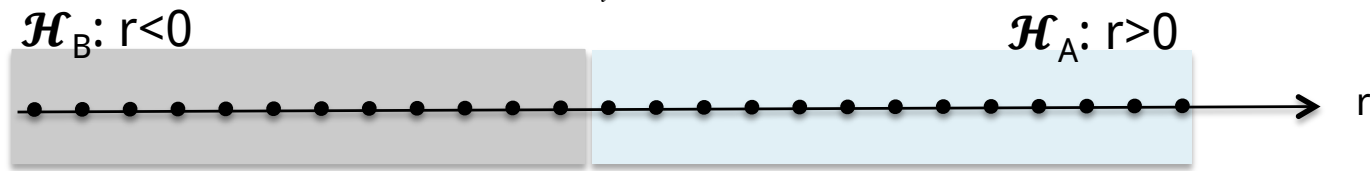


$$T = 0: H_E \cong \sum_{r>0} t \alpha r (\hat{c}_r^\dagger \hat{c}_{r+1} + h.c.)$$

$$T > 0: H_E \cong \sum_{r>0} t \beta (\hat{c}_r^\dagger \hat{c}_{r+1} + h.c.)$$

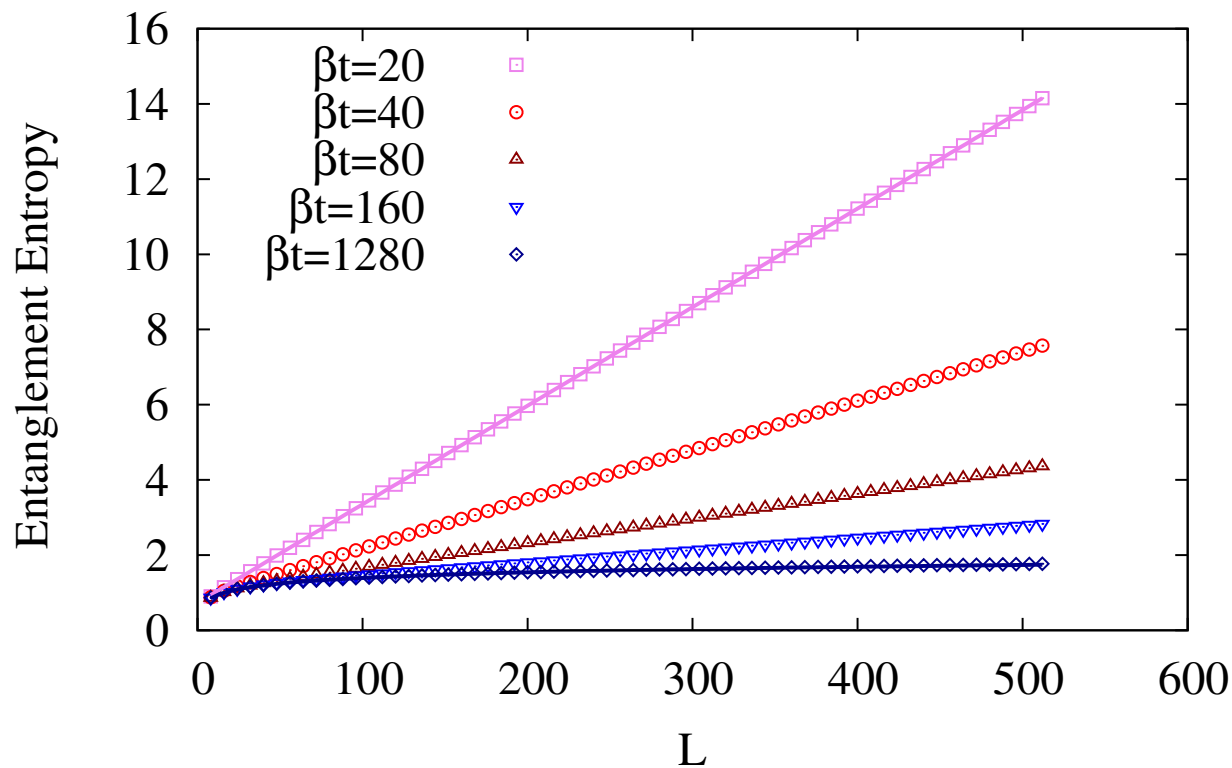
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Entanglement entropy = Von Neumann entropy of H_E



$T > 0$: $a + b L$

Volume law

$T = 0$: $a + b \log(L)$

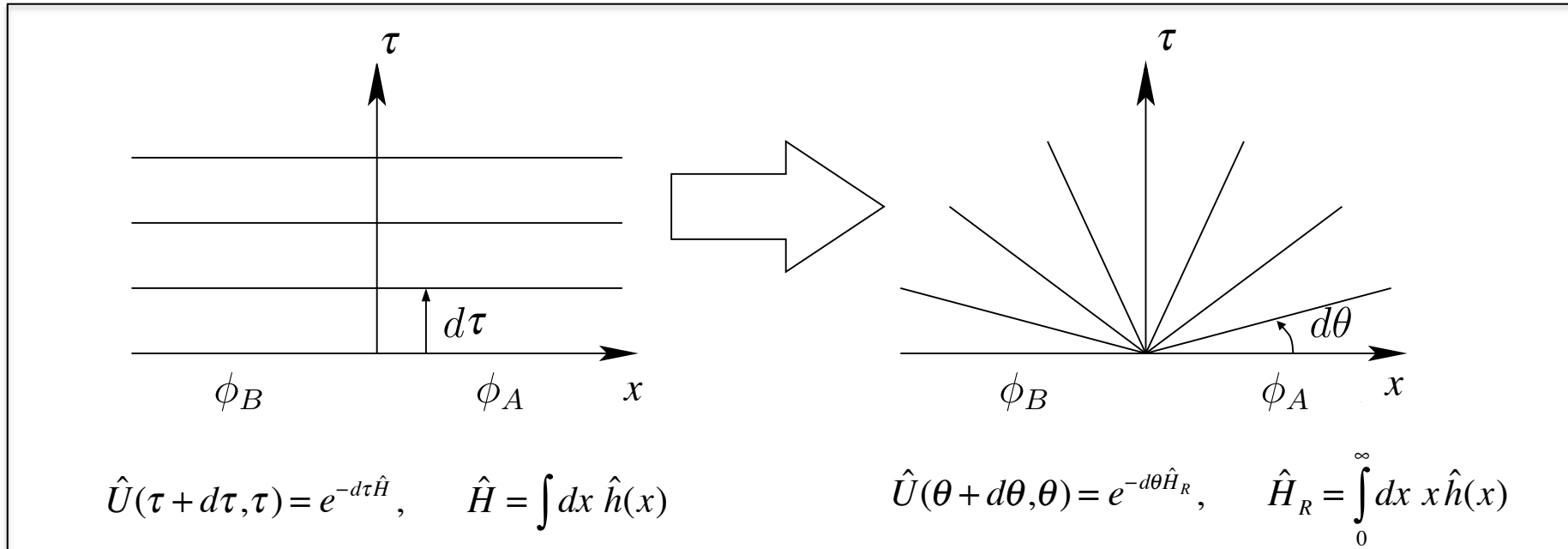
Area law with additive log correction.

Pasquale Calabrese and John Cardy
J. Stat. Mech.: Theor. Exp. (2004) P06002

The Rindler Hamiltonian

$$\langle \psi_0 | \phi_B \phi_A \rangle = \lim_{\beta \rightarrow \infty} \langle \psi_T | e^{-\beta \hat{H}} | \phi_B \phi_A \rangle = \langle \phi_B | e^{-\pi \hat{H}_R} | \phi_A \rangle$$

Lorentz invariance required!

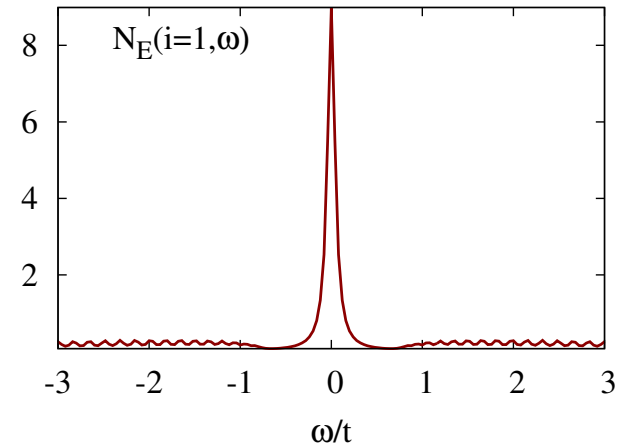
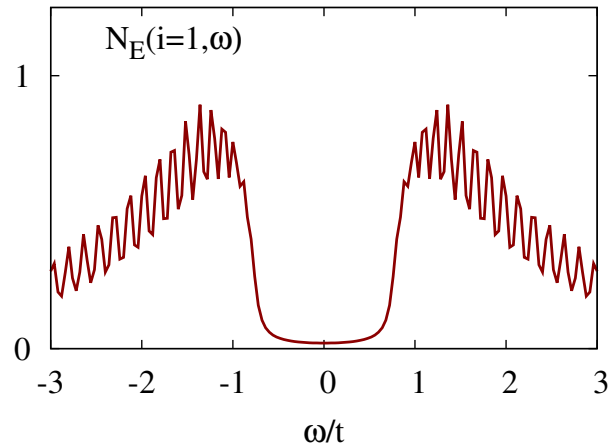
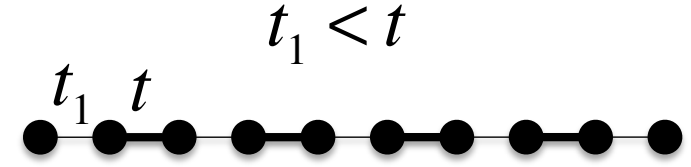
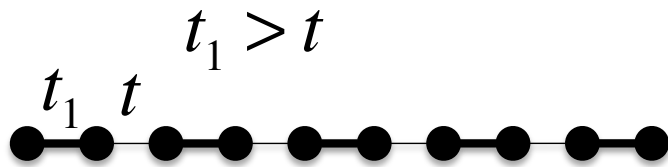
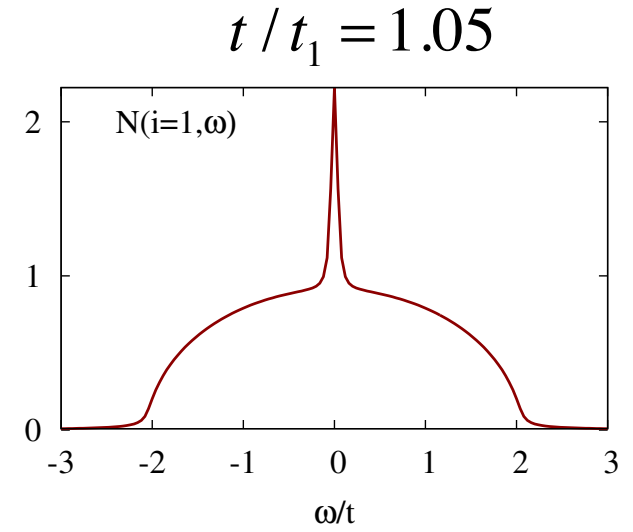
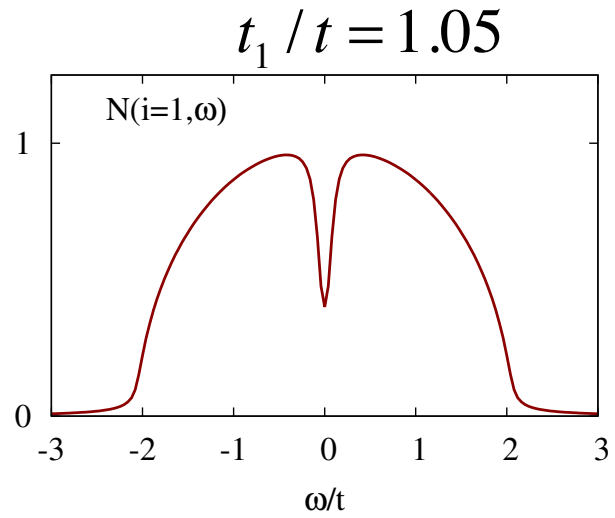


$$\langle \phi'_A | \hat{\rho}_A | \phi_A \rangle = \sum_{|\phi_B\rangle} \langle \phi_B \phi'_A | \psi_0 \rangle \langle \psi_0 | \phi_B \phi_A \rangle = \sum_{|\phi_B\rangle} \langle \phi'_A | e^{-\pi \hat{H}_R} | \phi_B \rangle \langle \phi_B | e^{-\pi \hat{H}_R} | \phi_A \rangle = \langle \phi'_A | e^{-2\pi \hat{H}_R} | \phi_A \rangle$$

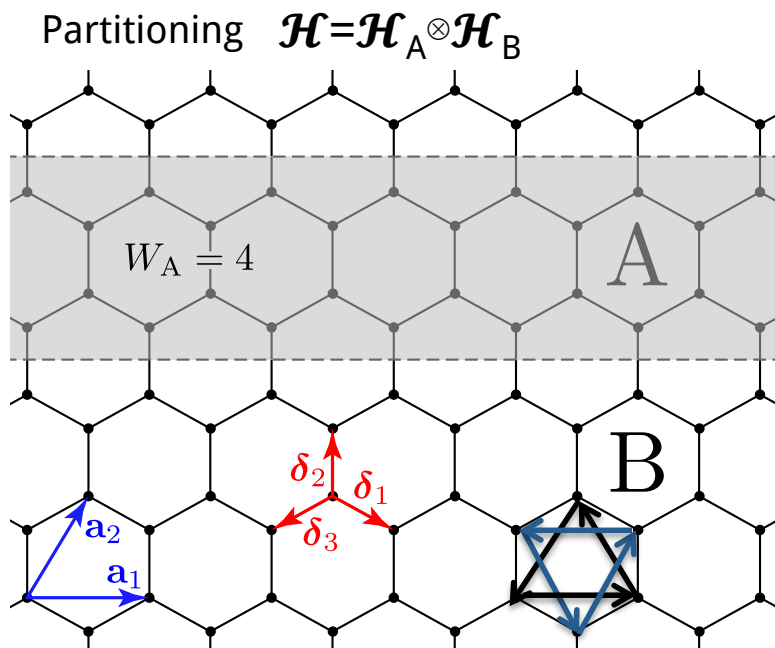
$$\hat{\rho}_A = e^{-2\pi \hat{H}_R}$$

$$\hat{H}_E = 2\pi \hat{H}_R = 2\pi \int_0^\infty dx x \hat{h}(x)$$

Detecting topological states with entanglement spectrum.



Entanglement spectrum for non-interacting topological insulators.

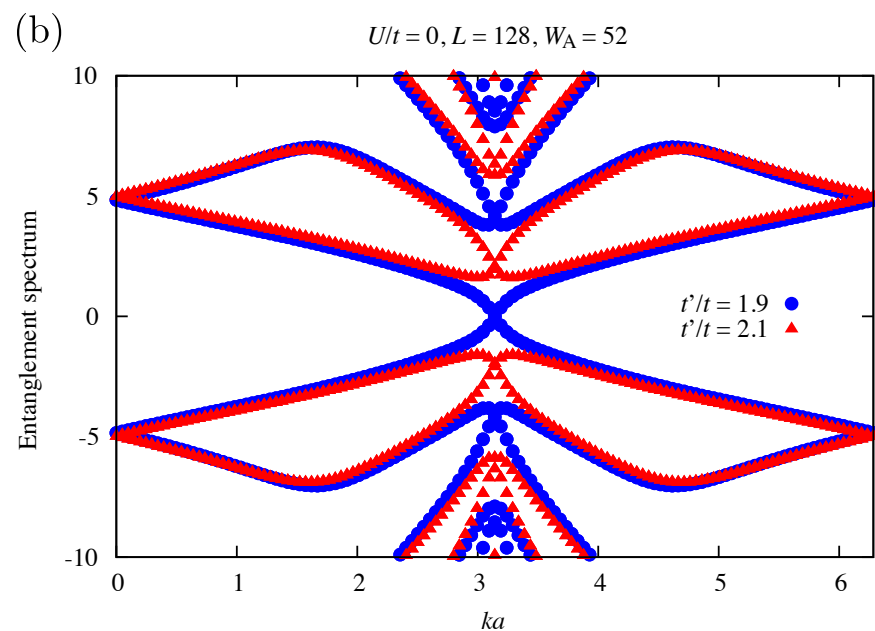
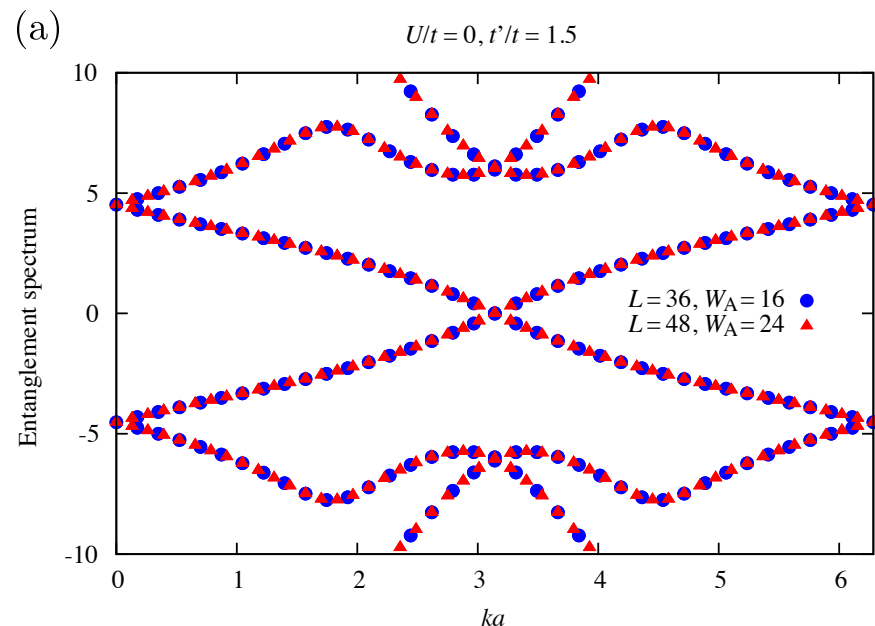


$$\hat{H}_{DKM} = \sum_{i,j} \hat{c}_i^\dagger (t_{i,j} + i\lambda_{i,j} \cdot \sigma) \hat{c}_j^\dagger$$

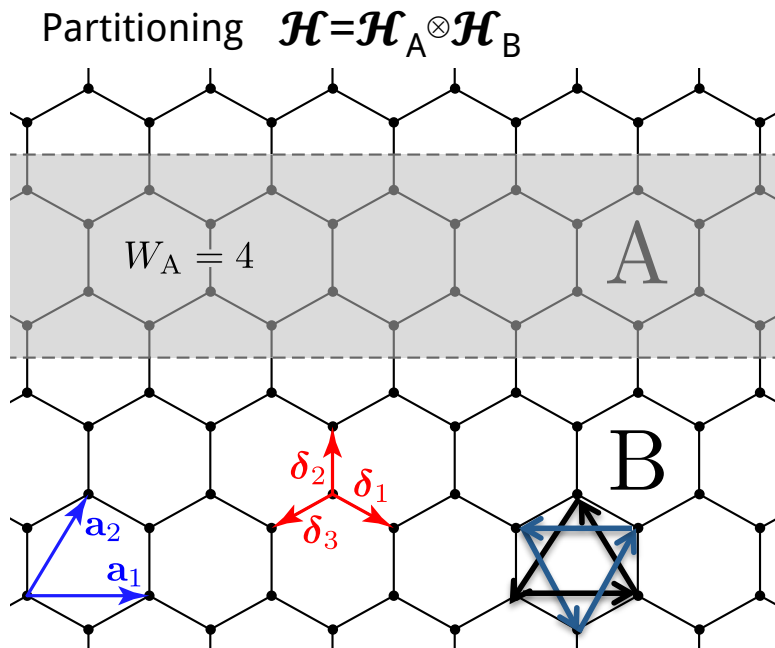
$$t_{ij} = \begin{cases} -t & \text{if } i - j = \pm\delta_2, \pm\delta_3 \\ -t' & \text{if } i - j = \pm\delta_1 \\ 0 & \text{otherwise} \end{cases}$$

$$\vec{i} \rightarrow \vec{j} = \lambda i (\hat{c}_i^\dagger \sigma_z \hat{c}_j - \hat{c}_j^\dagger \sigma_z \hat{c}_i)$$

Topological phase transition @ $t'/t = 2$



Entanglement spectrum for non-interacting topological insulators.

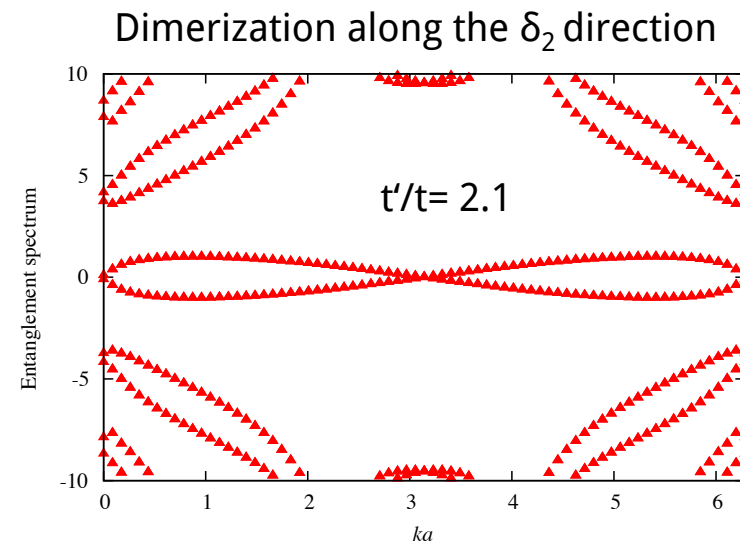
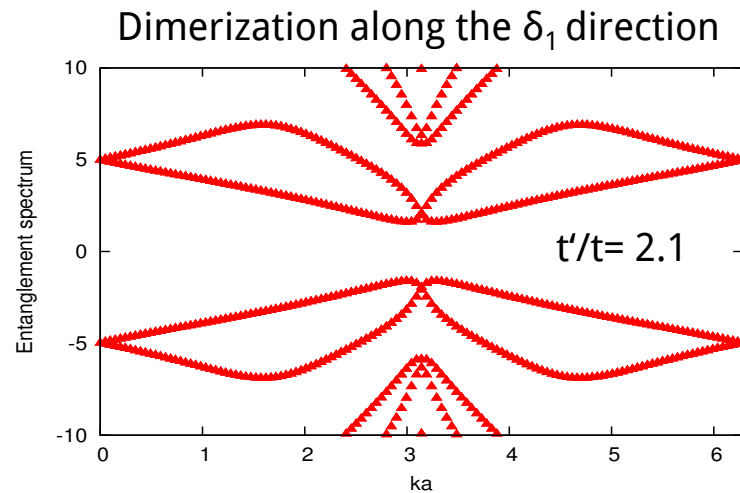


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Topological phase transition @ $t'/t=2$



See also

A, Chandran, V. Khemani, S. L. Sondhi Phys. Rev. Lett. 113, 060501 (2014)

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F. Parisen Toldin



T. Lang

Auxiliary field QMC. BSS: R. Blankenbecler, D. J. Scalapino, R. L. Sugar (1981)

$$\text{Tr} e^{-\beta \hat{H}} \propto \int D\{\Phi(\mathbf{i}, \tau)\} e^{-S(\{\Phi(\mathbf{i}, \tau)\})}$$

Trotter, Hubbard-Stratonovich

MC importance
sampling

One body problem in
external field

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Trotter, Hubbard-Stratonovich

MC importance sampling

One body problem in external field

Example

For $\hat{H} = \hat{H}_{KM} + \frac{1}{4} \sum_{\mathbf{i}, \mathbf{j}} V_{\mathbf{i}, \mathbf{j}} (\hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{i}} - 1)(\hat{c}_{\mathbf{j}}^{\dagger} \hat{c}_{\mathbf{j}} - 1), \quad \hat{c}_{\mathbf{i}}^{\dagger} = (\hat{c}_{\mathbf{i}, \uparrow}^{\dagger}, \hat{c}_{\mathbf{i}, \downarrow}^{\dagger})$

$$S(\{\Phi(\mathbf{i}, \tau)\}) = \sum_{\mathbf{i}, \mathbf{j}, \tau} \Delta\tau \Phi(\mathbf{i}, \tau) V_{\mathbf{i}, \mathbf{j}}^{-1} \Phi(\mathbf{j}, \tau) - \ln \text{Tr} \left[\prod_{\tau=1}^{L_{\tau}} e^{-\Delta\tau \hat{H}_{KM}} e^{-\Delta\tau \sum_{\mathbf{i}} \Phi(\mathbf{i}, \tau) [\hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{i}} - 1]} \right]$$

- The action is real! → positive weights
(U(1) spin symmetry, particle-hole symmetry, V positive definite)
- Scaling βN^3

Measuring observables.

$$\frac{\text{Tr} \left[e^{-\beta \hat{H}} \hat{c}_x^\dagger \hat{c}_y \right]}{\text{Tr} e^{-\beta \hat{H}}} = \int D\Phi P(\Phi) G_{x,y}(\Phi)$$

$$P(\Phi) = \frac{e^{-S(\Phi)}}{\int D\Phi e^{-S(\Phi)}}, \quad G(\Phi) = (1 + B_{L_t} \cdots B_1)^{-1}$$

Wicks theorem holds for a given field configuration \rightarrow

Any equal time observable can be computed from G

A different way of writing Wick's theorem. T. Grover Phys. Rev. Lett., 111, 130402, (2013).

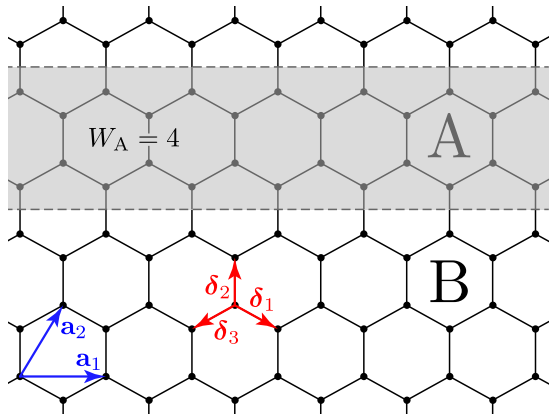
$$\hat{\rho} \equiv \frac{e^{-\beta \hat{H}}}{Z} = \int d\Phi P(\Phi) \hat{\rho}(\Phi), \quad \hat{\rho}(\Phi) = \det[1 - G(\Phi)] e^{-\hat{c}^\dagger \ln[G^{-1}(\Phi) - 1] \hat{c}}$$

$$\rightarrow \int d\Phi P(\Phi) \text{Tr} [\hat{\rho}(\Phi) \hat{O}] = \langle \hat{O} \rangle$$

For all equal time observables.

Renyi entanglement entropies

T. Grover Phys. Rev. Lett., 111, 130402, (2013).



$$\hat{\rho}_A = \text{Tr}_B \hat{\rho} \equiv \int d\Phi P(\Phi) \hat{\rho}_A(\Phi)$$

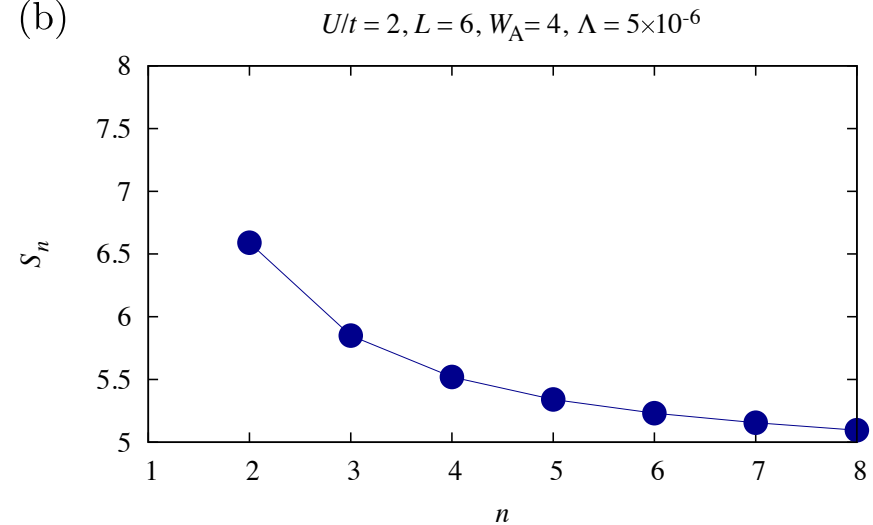
n-replicas

$$\text{Tr} \hat{\rho}_A^n = \int \overbrace{d\Phi^1 \dots d\Phi^n}^{\text{n-replicas}} P(\Phi^1) \dots P(\Phi^n) \text{Tr} [\hat{\rho}_A(\Phi^1) \dots \hat{\rho}_A(\Phi^n)]$$

$$S_n = -\frac{1}{n-1} \ln \text{Tr} \hat{\rho}_A^n$$

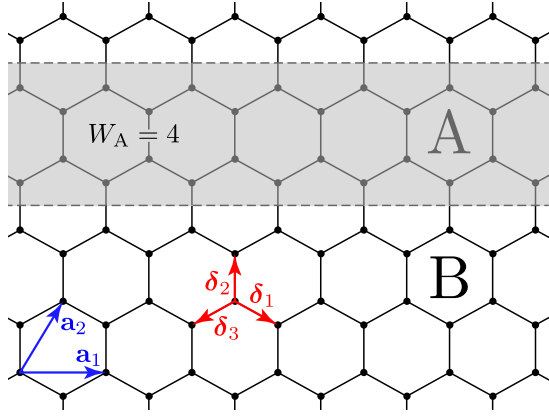
F. F. Assaad, T. C. Lang, and F. Parisen Toldin
Phys. Rev. B, 89, 125121, (2014)

(b)



Entanglement Hamiltonian

T. Grover Phys. Rev. Lett., 111, 130402, (2013).



$$\hat{\rho}_A = e^{-\hat{H}_E} = \text{Tr}_B \hat{\rho} \equiv \int d\Phi P(\Phi) \hat{\rho}_A(\Phi),$$

$$\text{with } \hat{\rho}_A(\Phi) = \underbrace{\det[1 - G_A(\Phi)]}_{\equiv e^{-\alpha(\Phi)}} e^{-\hat{c}^\dagger \ln \left[\overbrace{G_A^{-1}(\Phi) - 1}^{\equiv h(\Phi)} \right] \hat{c}}$$

Cumulant expansion:

$$\hat{H}_E = \sum_{x,y} t_{x,y} \hat{c}_x^\dagger \hat{c}_y + \sum_{x,y,w,z} U_{x,y,w,z} \hat{c}_x^\dagger \hat{c}_y \hat{c}_w^\dagger \hat{c}_z + \dots$$

$$t_{x,y} = \langle h(\Phi)_{x,y} \rangle - \left[\langle \alpha(\Phi) h(\Phi)_{x,y} \rangle - \langle \alpha(\Phi) \rangle \langle h(\Phi)_{x,y} \rangle \right]$$

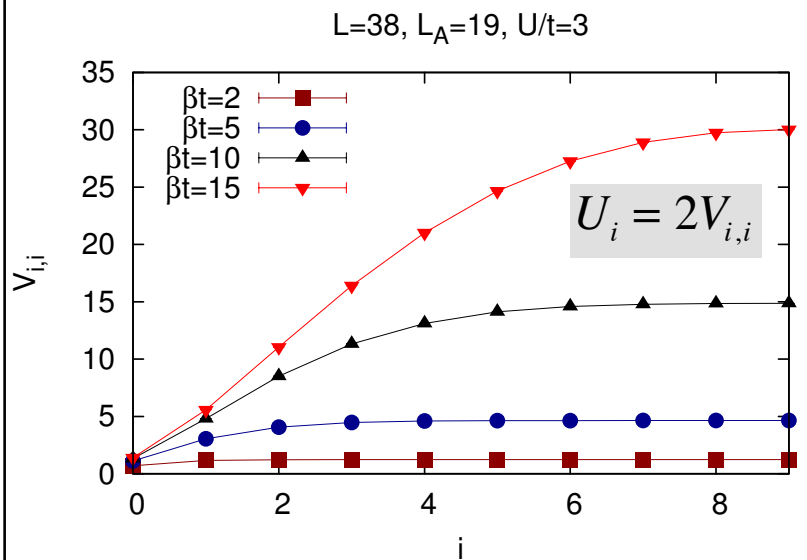
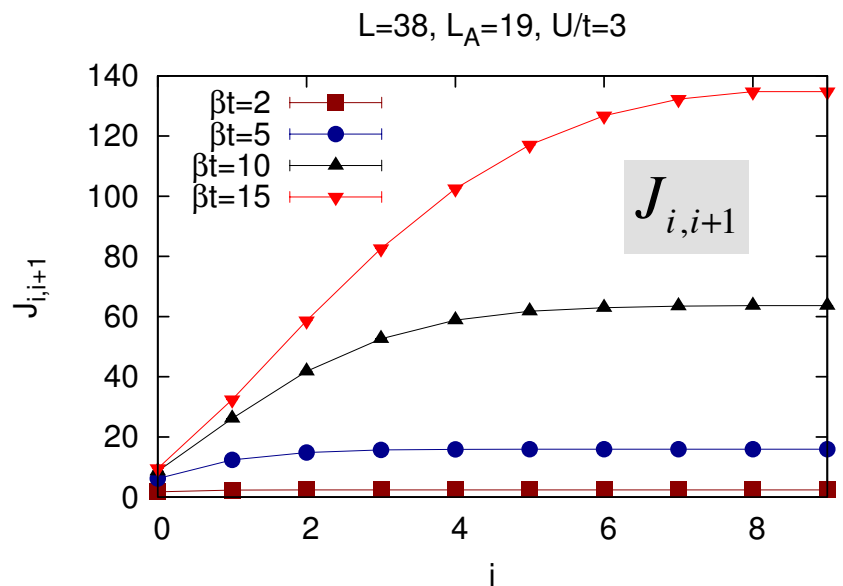
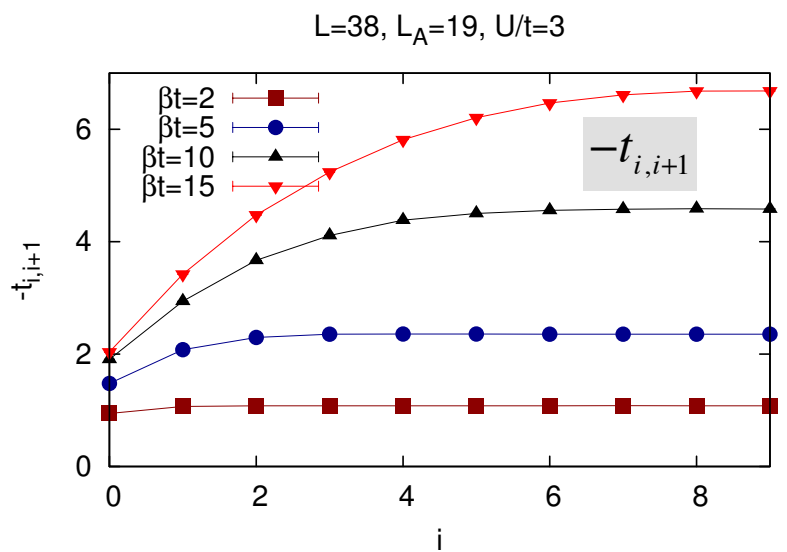
$$U_{x,y,w,z} = - \left[\langle h(\Phi)_{x,y} h(\Phi)_{w,z} \rangle - \langle h(\Phi)_{x,y} \rangle \langle h(\Phi)_{w,z} \rangle \right]$$

Note $\langle h(\Phi)_{x,y} \rangle = \int d\Phi P(\Phi) h(\Phi)_{x,y}$

1D Hubbard model @ $U/t = 3, \langle n \rangle = 1$

$$H_E = \sum_{i,n,\sigma} -t_{i,i+n} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+n,\sigma} + \hat{c}_{i+n,\sigma}^\dagger \hat{c}_{i,\sigma}) + \sum_{i,n} V_{i,i+n} \hat{n}_i \hat{n}_{i+n} + \sum_{i,n} \frac{-J_{i,i+n}}{4} (D_{i,i+n}^\dagger D_{i,i+n} + D_{i,i+n} D_{i,i+n}^\dagger) + \dots$$

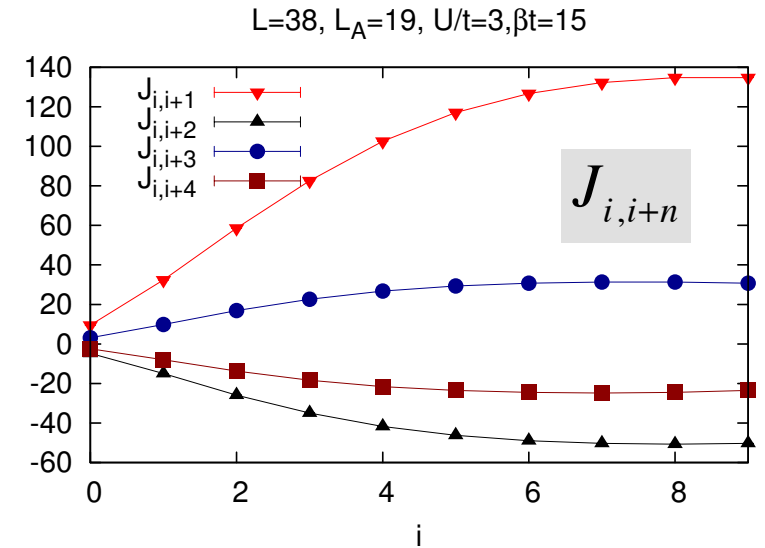
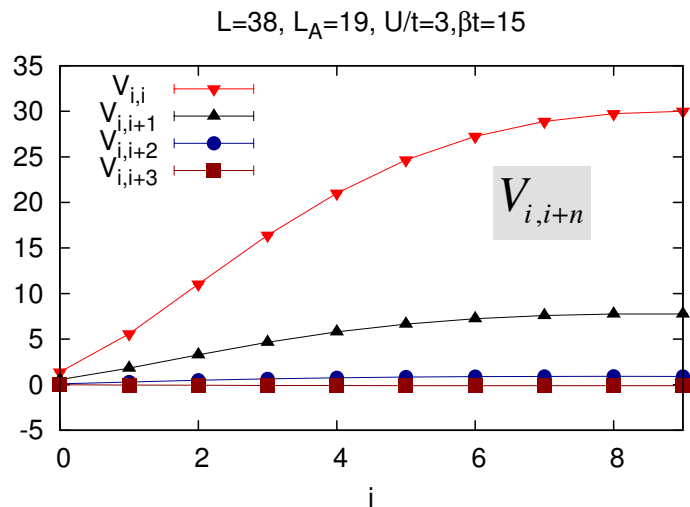
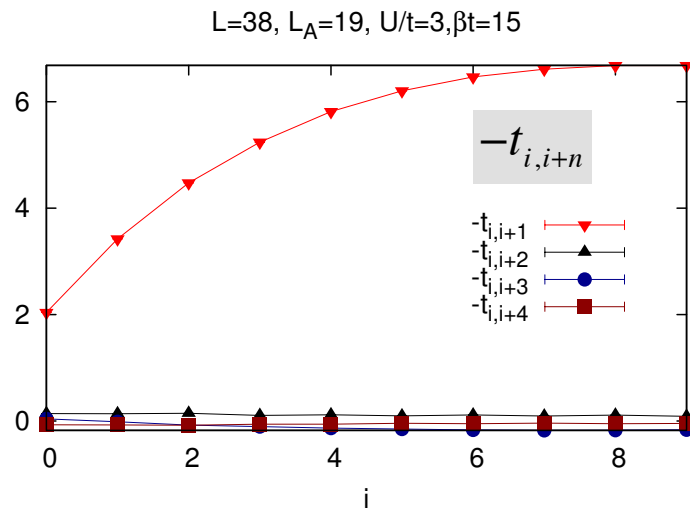
$$D_{i,i+n}^\dagger = \sum_{\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i+n,\sigma}$$



1D Hubbard model @ $U/t = 3, \langle n \rangle = 1$

$$H_E = \sum_{i,n,\sigma} -t_{i,i+n} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+n,\sigma} + \hat{c}_{i+n,\sigma}^\dagger \hat{c}_{i,\sigma}) + \sum_{i,n} V_{i,i+n} \hat{n}_i \hat{n}_{i+n} + \sum_{i,n} \frac{-J_{i,i+n}}{4} (D_{i,i+n}^\dagger D_{i,i+n} + D_{i,i+n} D_{i,i+n}^\dagger) + \dots$$

$$D_{i,i+n}^\dagger = \sum_{\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i+n,\sigma}$$



Entanglement spectrum

F. F. Assaad, T. C. Lang, and F. Parisen Toldin Phys. Rev. B, 89, 125121, (2014)

$$\langle a_x^\dagger(\tau)a_y \rangle = \frac{\text{Tr}\left[e^{-(\beta-\tau)H} a_x^\dagger e^{-\tau H} a_y\right]}{\text{Tr}\left[e^{-\beta H}\right]} \quad \rightarrow \quad \langle a_x^\dagger(\tau)a_x \rangle = \int d\omega \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}} A(x,\omega)$$

$$A(x,\omega) = \frac{1}{Z} \sum_{n,m} \left(e^{-\beta E_n} + e^{-\beta E_m} \right) \left| \langle n | a_x^\dagger | m \rangle \right|^2 \delta(\omega - E_m + E_n)$$

$$\hat{\rho}_A = e^{-\hat{H}_E}$$

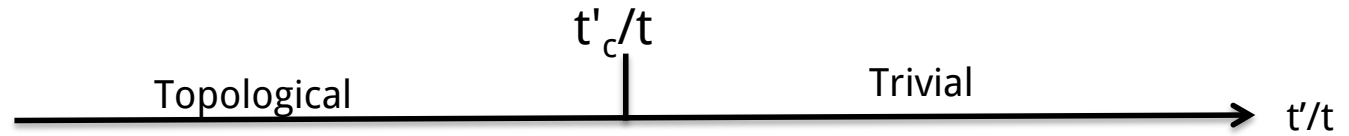
$$\langle a_x^\dagger(\tau_E)a_y \rangle_E = \frac{\text{Tr}\left[\hat{\rho}_A^{n-\tau_E} a_x^\dagger \hat{\rho}_A^{\tau_E} a_y\right]}{\text{Tr}\left[\hat{\rho}_A^n\right]} \quad \rightarrow \quad \langle a_x^\dagger(\tau_E)a_x \rangle_E = \int d\omega \frac{e^{-\tau_E\omega}}{1+e^{-n\omega}} A^E(x,\omega)$$

Note: n, τ_E are natural numbers \rightarrow restricted to low energy sector of the entanglement spectrum.

Entanglement spectrum

F. F. Assaad, T. C. Lang, and F. Parisen Toldin Phys. Rev. B, 89, 125121, (2014)

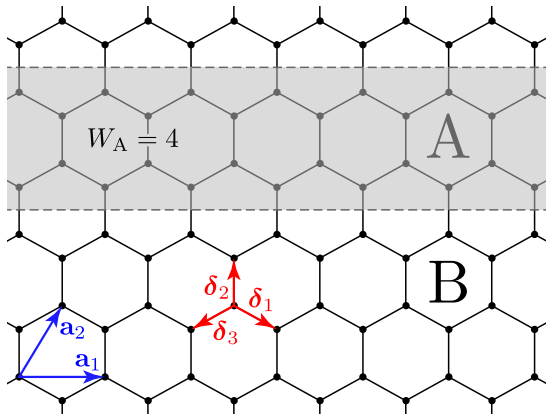
Example: Single particle entanglement spectral function for dimerized Kane-Mele Hubbard model.



Dimerization along the δ_1 direction

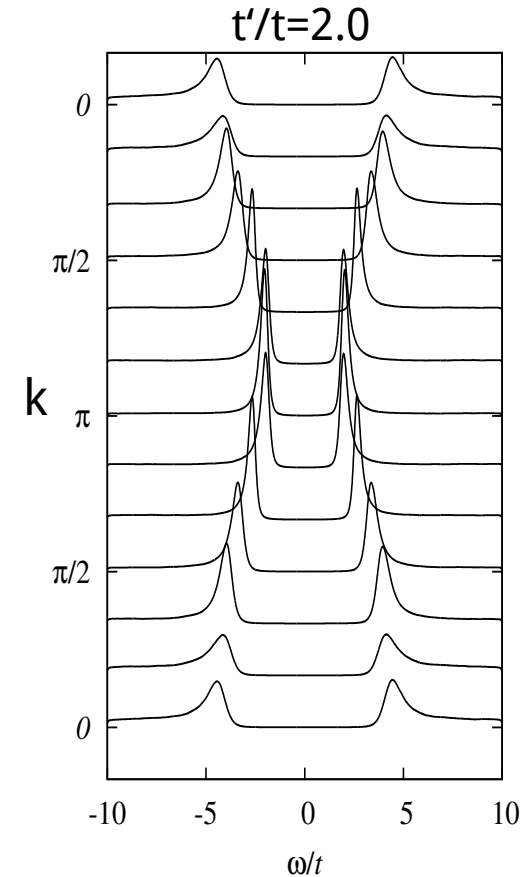
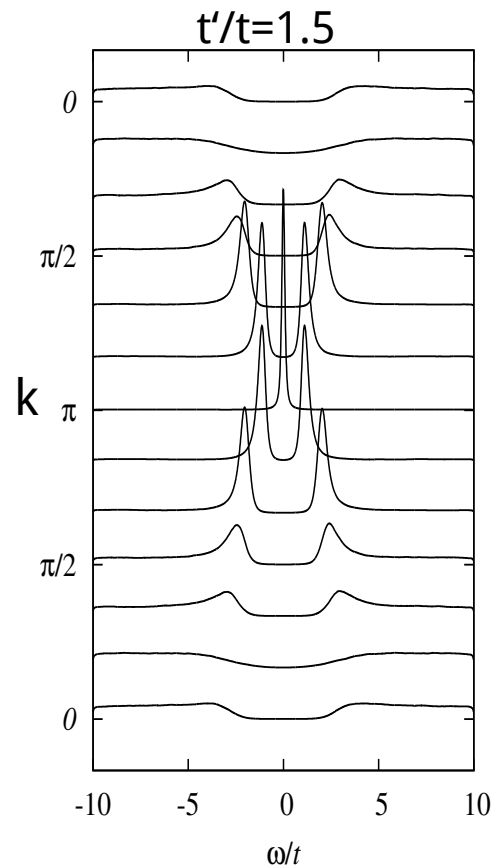
$$A_{1,1}^E(k, \omega) @ n = 8$$

$U/t = 2, \lambda/t = 0.2$



@ $U/t=2$: $1.95 < t'_c/t < 2$

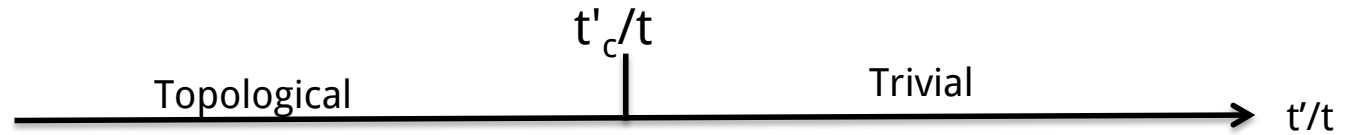
T. C. Lang, A. M. Essin, V. Gurarie,
and S. Wessel,
Phys. Rev. B 87, 205101 (2013).



Entanglement spectrum

F. F. Assaad, T. C. Lang, and F. Parisen Toldin Phys. Rev. B, 89, 125121, (2014)

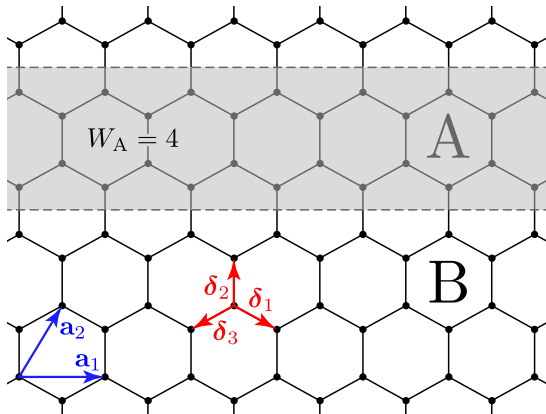
Example: Single particle entanglement spectral function for dimerized Kane-Mele Hubbard model.



Dimerization along the δ_2 direction

$$A_{1,1}^E(k, \omega) @ n = 8$$

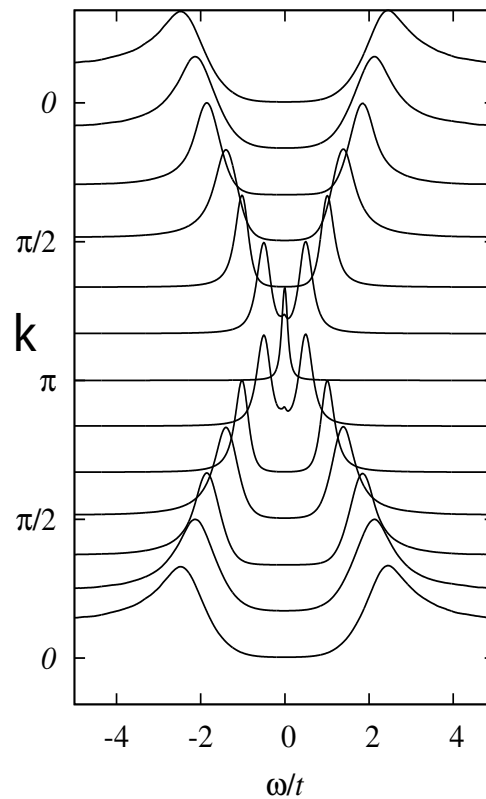
$U/t = 2, \lambda/t = 0.2$



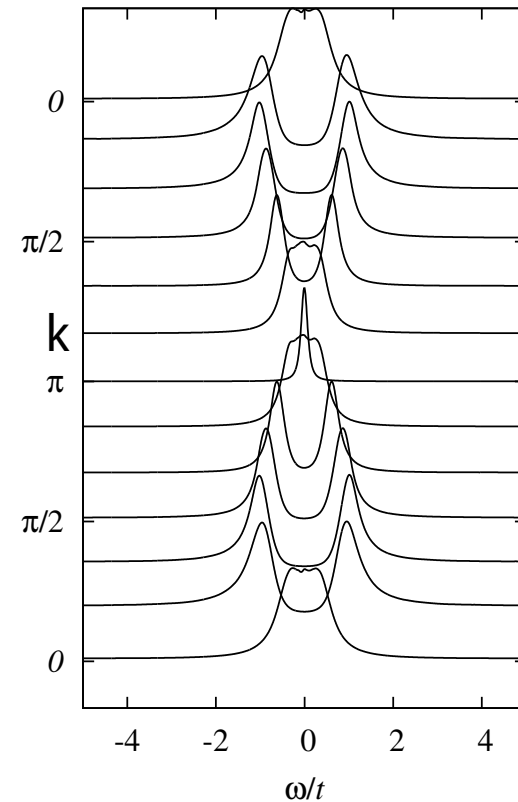
@ $U/t=2$: $1.95 < t'_c/t < 2$

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$t'/t=1.5$



$t'/t=2.0$



Limitations of the Gaussian (or weak coupling) approach.

$$\hat{\rho}_A = \int d\Phi P(\Phi) \hat{\rho}_A(\Phi)$$

→ Fluctuations! e.g n=2

$$\text{Tr} \hat{\rho}_A^2 = \int d\Phi^1 d\Phi^2 \overbrace{P(\Phi^1)P(\Phi^2)}^{\text{Sample}} \overbrace{\text{Tr}_A [\hat{\rho}_A(\Phi^1) \hat{\rho}_A(\Phi^2)]}^{\text{Measure}}$$

$$\frac{\langle \Delta \text{Tr} [\hat{\rho}_A(\Phi^1) \hat{\rho}_A(\Phi^2)] \rangle}{\langle \text{Tr} [\hat{\rho}_A(\Phi^1) \hat{\rho}_A(\Phi^2)] \rangle} \approx \frac{b / \sqrt{T_{CPU}}}{e^{-a\partial_A}} \ll 1 \quad T_{CPU} \gg b^2 e^{2a\partial_A} \quad \boxtimes$$

→ Entanglement spectrum

$$\langle a_x^\dagger(\tau_E) a_y \rangle_E = \frac{\text{Tr}_A [\hat{\rho}_A^{n-\tau_E} a_x^\dagger \hat{\rho}_A^{\tau_E} a_y]}{\text{Tr}_A [\hat{\rho}_A^n]} \quad \boxtimes$$

$$\text{Tr} \hat{\rho}_A^n = \int d\Phi^1 \dots d\Phi^n \underbrace{P(\Phi^1) \dots P(\Phi^n)}_{\text{Sample}} \overbrace{\text{Tr}_A [\hat{\rho}_A(\Phi^1) \dots \hat{\rho}_A(\Phi^n)]}^{\text{Is positive}}$$

→ Identical to replica approach

FFA, PRB 91, 125146 (2015)

→ Entanglement Hamiltonian with cumulant expansion



Entanglement Hamiltonian and spectra from quantum Monte Carlo simulations of interacting fermions.

Fakher F. Assaad (KITP, June 23rd 2015)

Organization

- Introduction: Entanglement Hamiltonian and spectra for free electrons.
- QMC
 - Weak coupling approaches → Gaussian representation of reduced density matrix
 - Strong coupling approaches → Replica
- Conclusions



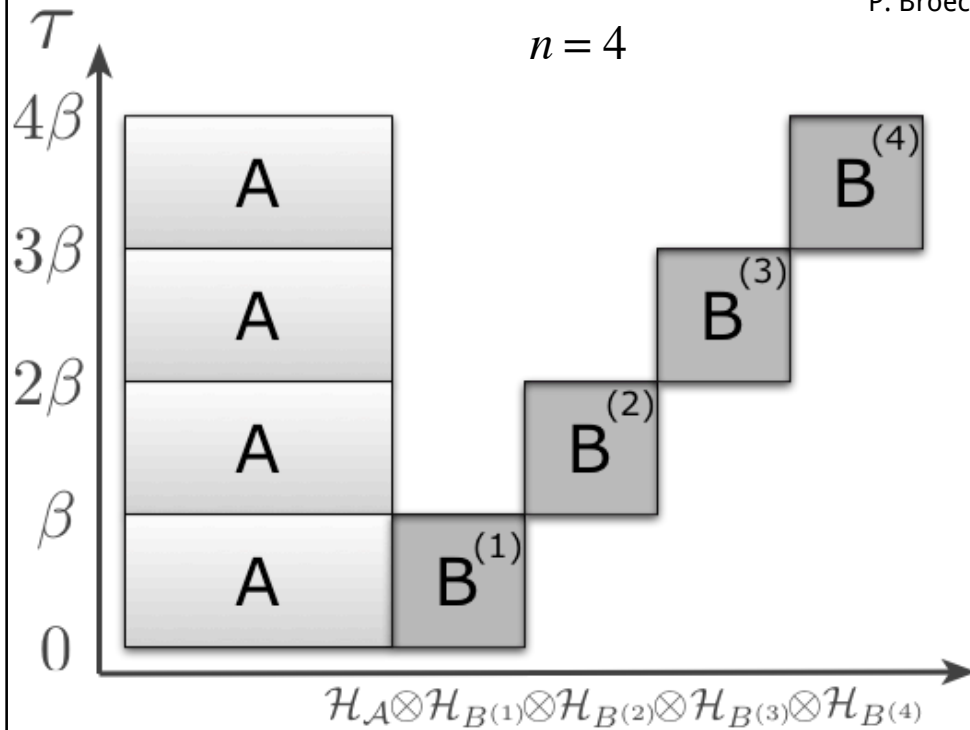
F. Parisen Toldin



T. Lang

Entanglement spectrum for strongly correlated electrons

M. B. Hastings, I. Gonzalez, A. B. Kallin, and R. G. Melko, Phys. Rev. Lett, 157201, (2010).
 P. Broecker and S. Trebst. JSTAT, P08015, (2014).



Replica method: Hilbert space

$$\mathcal{H}_{\text{tot}} = \mathcal{H}_A \otimes \mathcal{H}_B^{(1)} \otimes \mathcal{H}_B^{(2)} \cdots \mathcal{H}_B^{(n)}$$

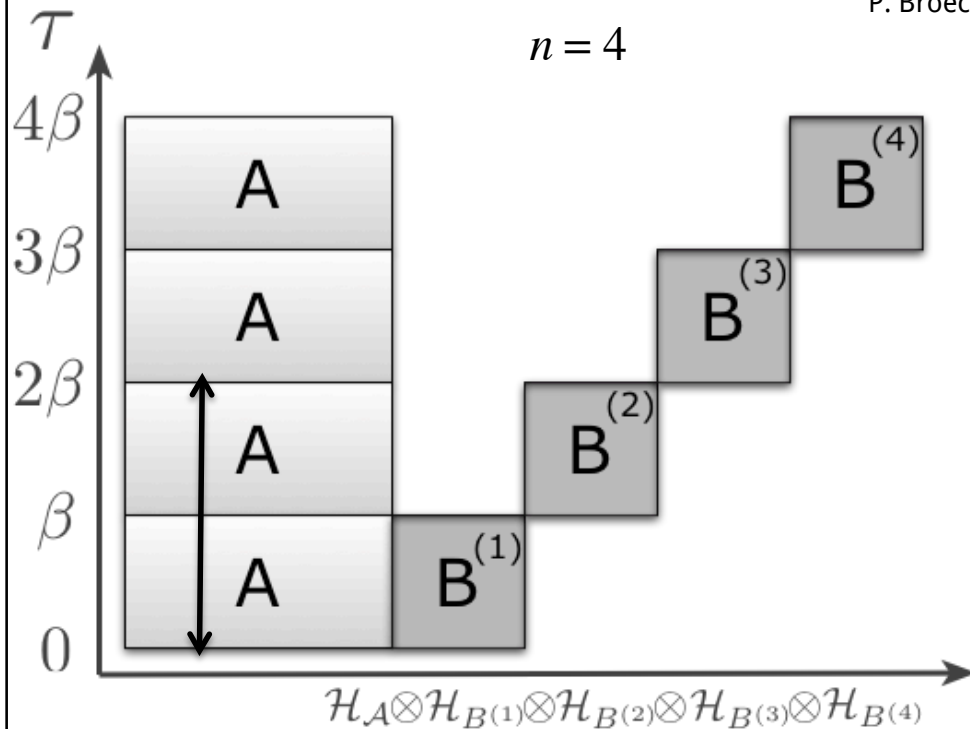
Time dependent Hamiltonian, $0 < \tau < n\beta$

$$\hat{H}(\tau) = \sum_{r=1}^n \Theta[\tau - (r-1)\beta] \Theta[r\beta - \tau] \hat{H}^{(r)}.$$

$\hat{H}^{(r)}$ Hamiltonian in Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B^{(r)}$

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$\hat{H}^{(r)}$ Hamiltonian in Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B^{(r)}$

$$\frac{\text{Tr}_{\mathcal{H}_{\text{tot}}} \left[\hat{U}(n\beta, \tau_E \beta) \hat{O}^\dagger \hat{U}(\tau_E \beta, 0) \hat{O} \right]}{\text{Tr}_{\mathcal{H}_{\text{tot}}} \left[\hat{U}(n\beta, 0) \right]} = \frac{\text{Tr}_{\mathcal{H}_A} \left[e^{-(n-\tau_E)\hat{H}_E} \hat{O}^\dagger e^{-\tau_E \hat{H}_E} \hat{O} \right]}{\text{Tr}_{\mathcal{H}_A} \left[e^{-n\hat{H}_E} \right]}$$

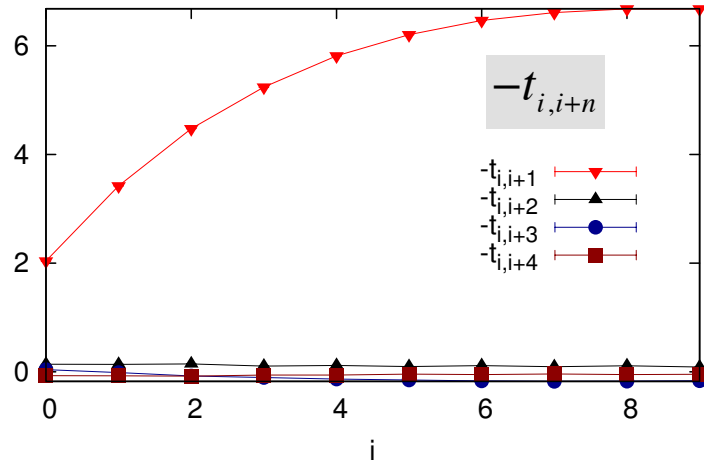
→ One can study equal time and dynamical properties of the entanglement Hamiltonian

One-dimensional Hubbard chain @ $U/t=3, \langle n \rangle=1$

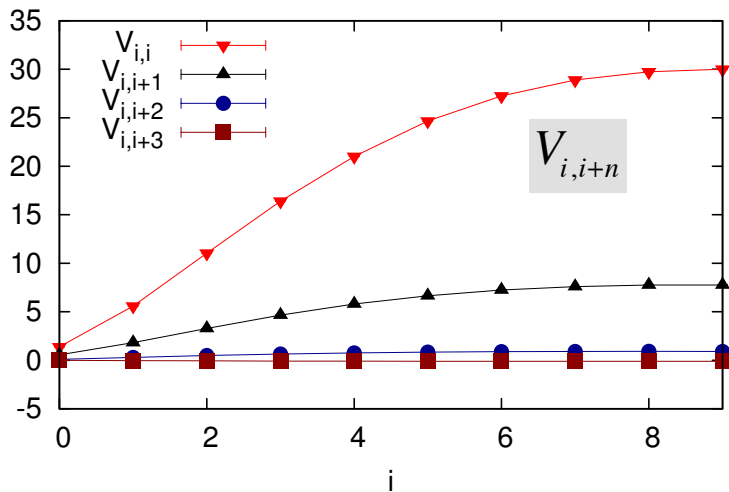
Cumulant expansion

$$H_E = \sum_{i,n,\sigma} -t_{i,i+n} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+n,\sigma} + \hat{c}_{i+n,\sigma}^\dagger \hat{c}_{i,\sigma} \right) + \sum_{i,n} V_{i,i+n} \hat{n}_i \hat{n}_{i+n} + \sum_{i,n} \frac{-J_{i,i+n}}{4} \left(D_{i,i+n}^\dagger D_{i,i+n} + D_{i,i+n} D_{i,i+n}^\dagger \right) + \dots$$

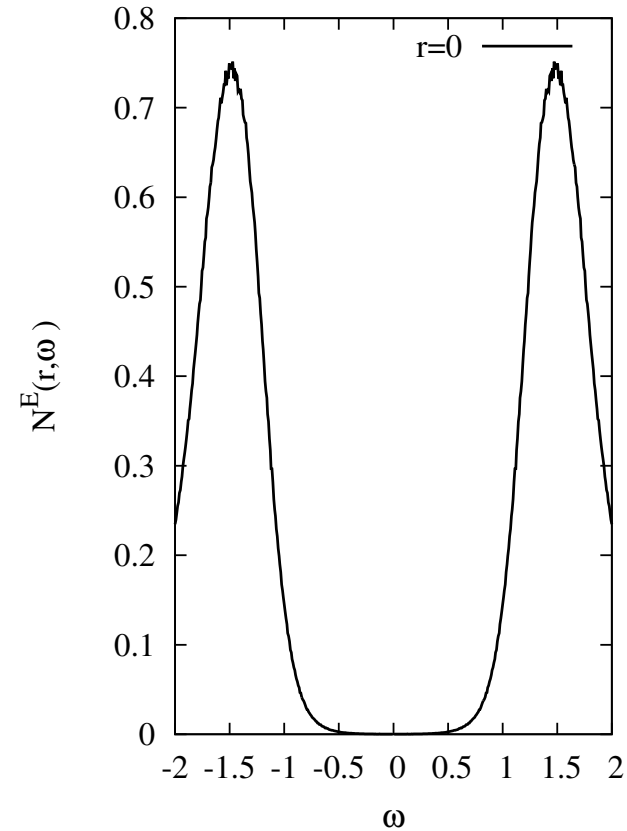
$L=38, L_A=19, U/t=3, \beta t=15$



$L=38, L_A=19, U/t=3, \beta t=15$



$L=38, L_A=19, \beta t=12, n=8$



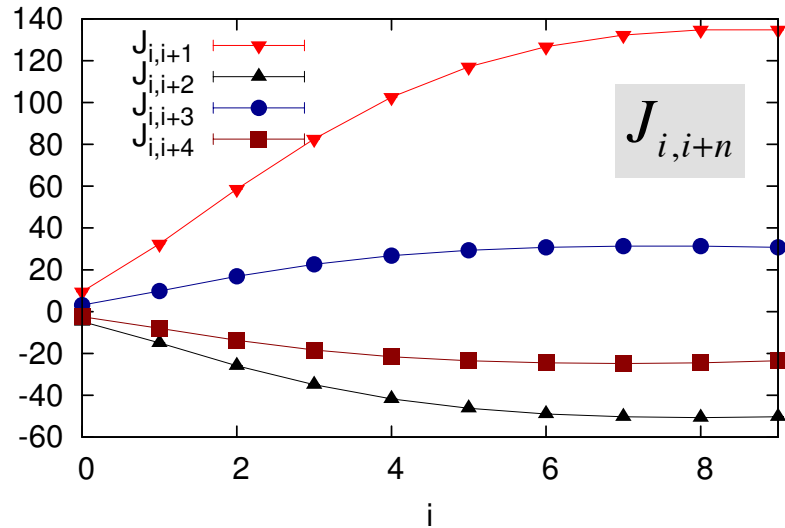
Single particle density of states of the entanglement Hamiltonian @ $r=0$. \rightarrow Gap @ $r > 0$ grows.
 \rightarrow Insulating state.

One-dimensional Hubbard chain @ $U/t=3, \langle n \rangle=1$

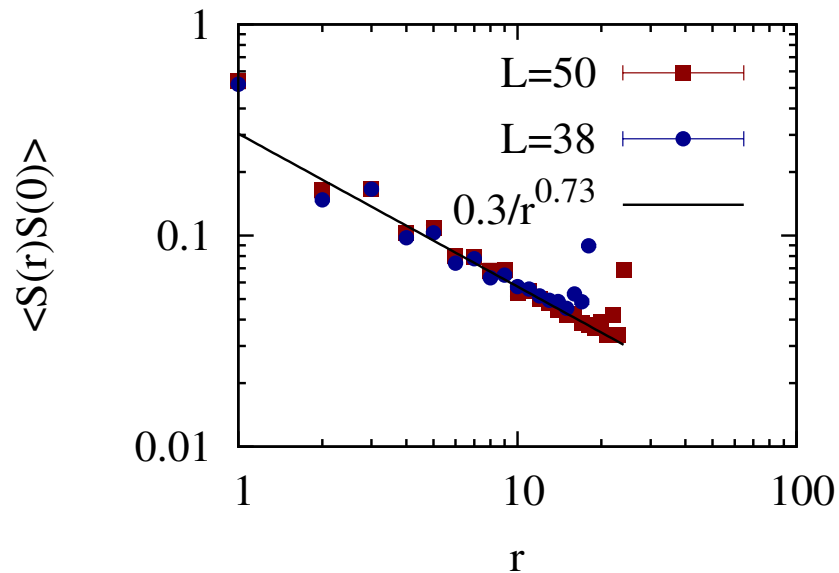
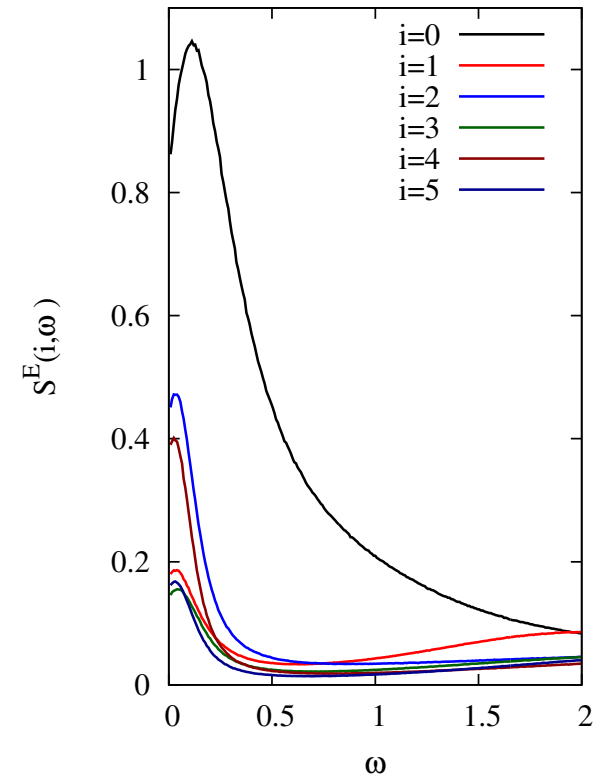
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$L=38, L_A=19, U/t=3, \beta t=15$

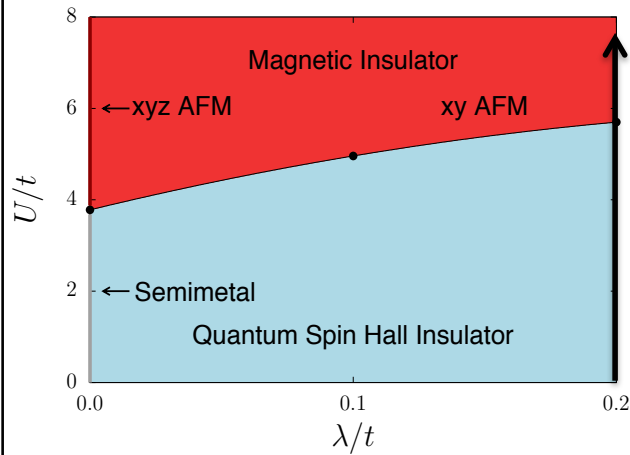


$L=38, L_A=19, \beta t=12, n=8$

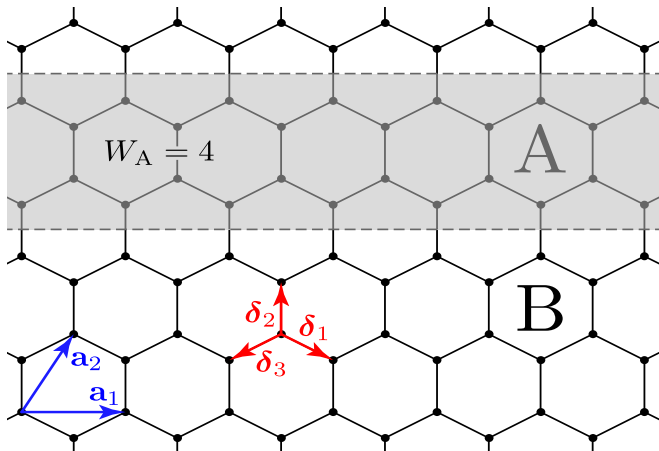
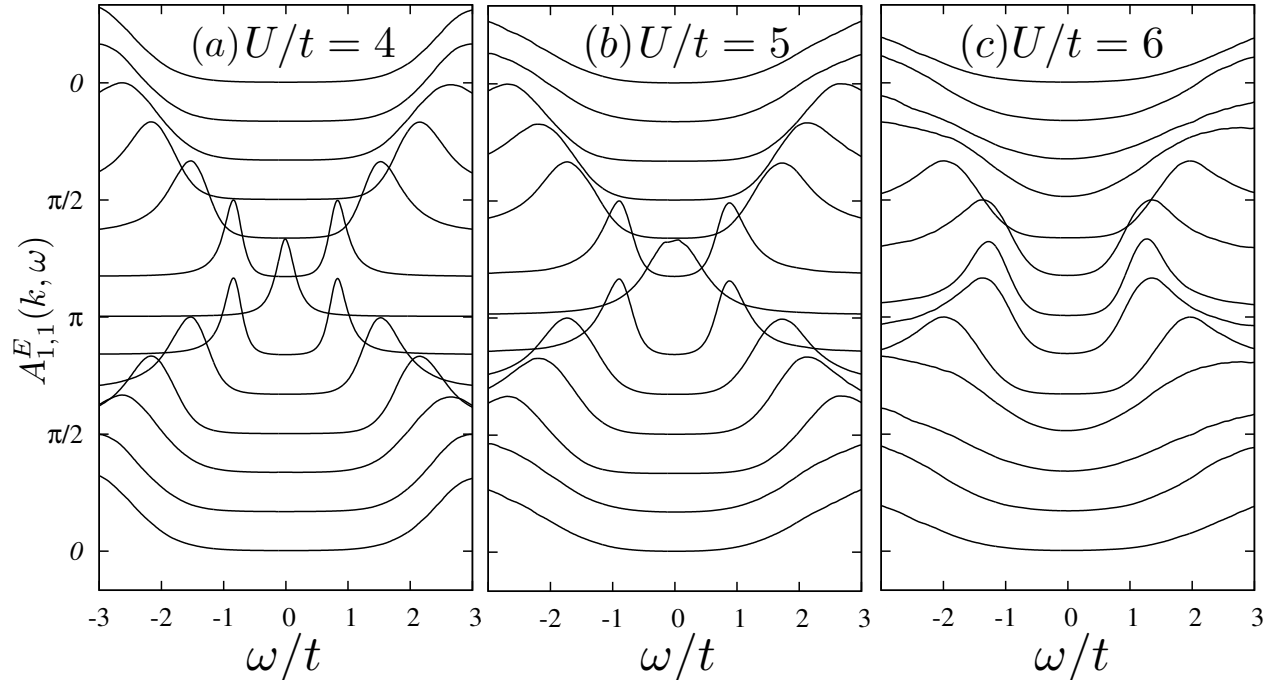


Local dynamical spin structure factor of the entanglement Hamiltonian \rightarrow Gapless spin excitations

Single-particle spectrum of the entanglement Hamiltonian



$$W_A = 16, \beta t = 4, n = 8 \quad 12 \times 12, \lambda/t = 0.2$$



$$\frac{\text{Tr}_{\mathcal{H}_A} \left[e^{-(n-\tau_E)\hat{H}_E} \hat{a}_{k,m}^\dagger e^{-\tau_E \hat{H}_E} \hat{a}_{k,m'} \right]}{\text{Tr}_{\mathcal{H}_A} \left[e^{-n\hat{H}_E} \right]}$$

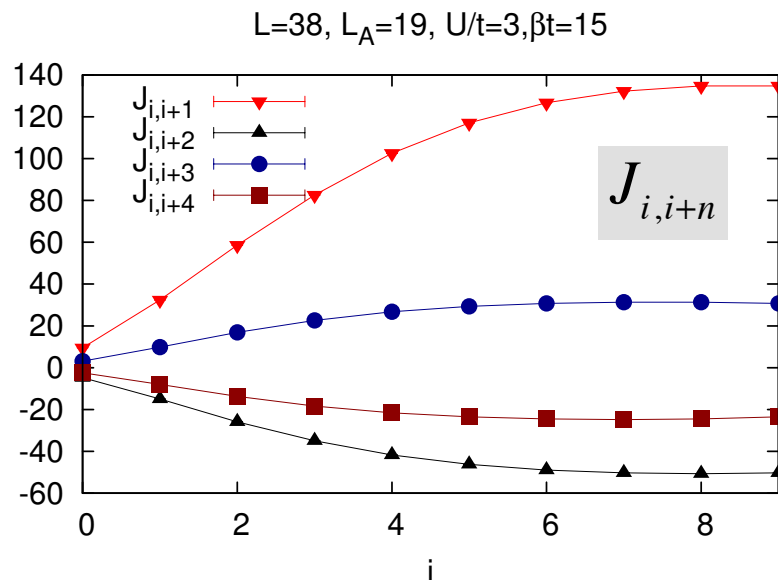
k : translation symmetry in a_1 , m : orbital index across partition A

Wick rotation (Stochastic MaxEnt) to produce spectral function

Summary

Part I Weak coupling methods. Direct calculation of entanglement Hamiltonian (cumulant expansion)

$$\begin{aligned}
 H_E = & \sum_{i,n,\sigma} -t_{i,i+n} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+n,\sigma} + \hat{c}_{i+n,\sigma}^\dagger \hat{c}_{i,\sigma} \right) + \\
 & \sum_{i,n} V_{i,i+n} \hat{n}_i \hat{n}_{i+n} + \\
 & \sum_{i,n} \frac{-J_{i,i+n}}{4} \left(D_{i,i+n}^\dagger D_{i,i+n} + D_{i,i+n} D_{i,i+n}^\dagger \right) + \dots
 \end{aligned}$$



Part II Method to compute entanglement spectrum of strongly correlated fermion systems with QMC.

