

第二届全国冷原子和量子信息青年学者学术讨论会



Fidelity susceptibility and quantum phase transitions

Speaker: Shi-Jian Gu

$$F(A, B) = \langle \Psi(A) | \Psi(B) \rangle$$

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Wen-Qiang Ning (Fudan U.)

Shuo Yang (ITP)



A physical phenomenon can be understood from different point of view.



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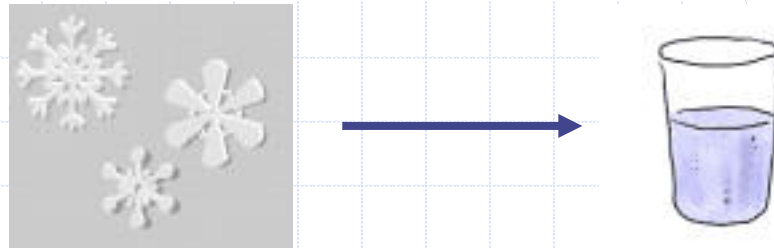
Content

- I. Introduction: quantum phase transition, fidelity in quantum information**
- II. Fidelity and dynamic structure factor in the ground state**
- III. Fidelity susceptibility and universality class**
- IV. Fidelity susceptibility in topological phase transitions.**
- V. Density-functional fidelity and reduced fidelity**
- VI. Summary**



Introduction: QPT

Thermal phase transitions: which is described by non-analytic behaviors of the thermal properties at the transition points, driven by thermal fluctuation.



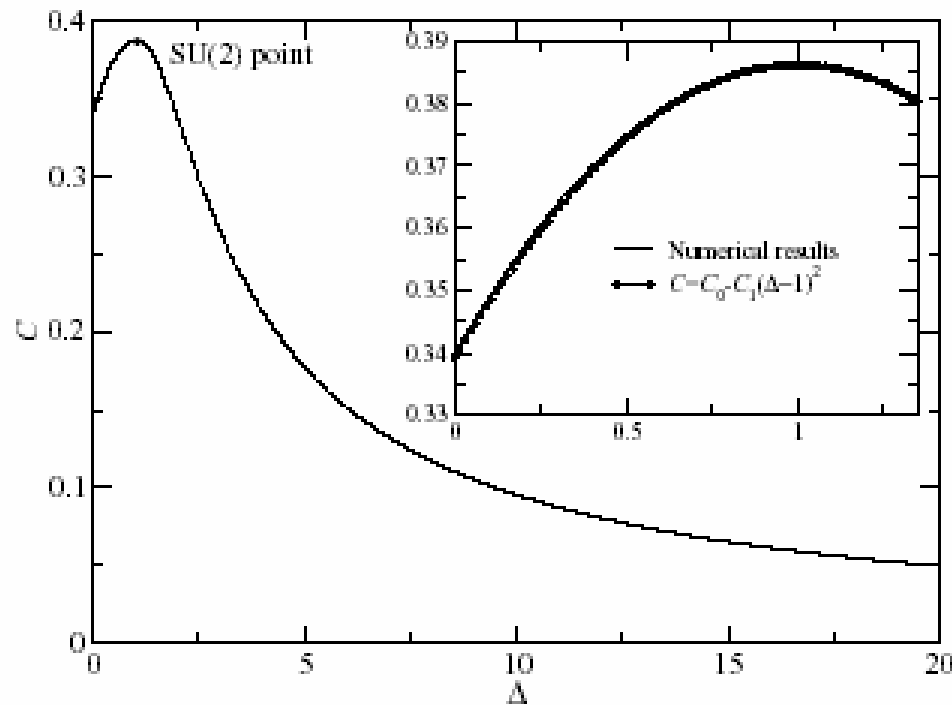
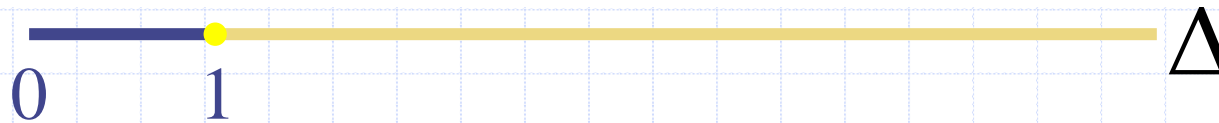
Quantum phase transitions: driven by the quantum fluctuations and are described by the non-analytic behaviors of the ground-state properties at the transition points.

- ❖ High T_c superconductor
- ❖ Mott-insulator transition in Hubbard model.



Introduction: QPT & quantum entanglement

$$\hat{H}_{XXZ} = \sum_i (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z);$$



$$C = C_0 - C_1(\Delta - 1)^2$$

$$C_0 = 2 \ln 2 - 1$$

$$C_1 = 2 \ln 2 - \frac{1}{2} - \frac{2}{\pi} - \frac{2}{\pi^2}$$

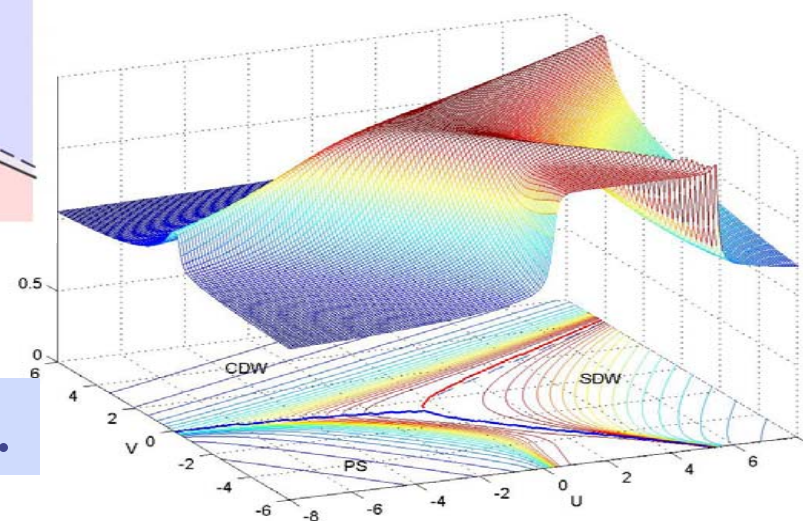
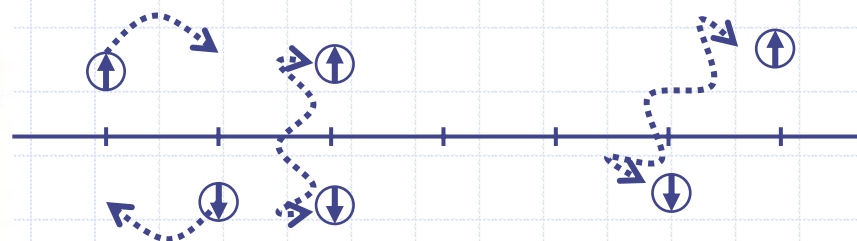
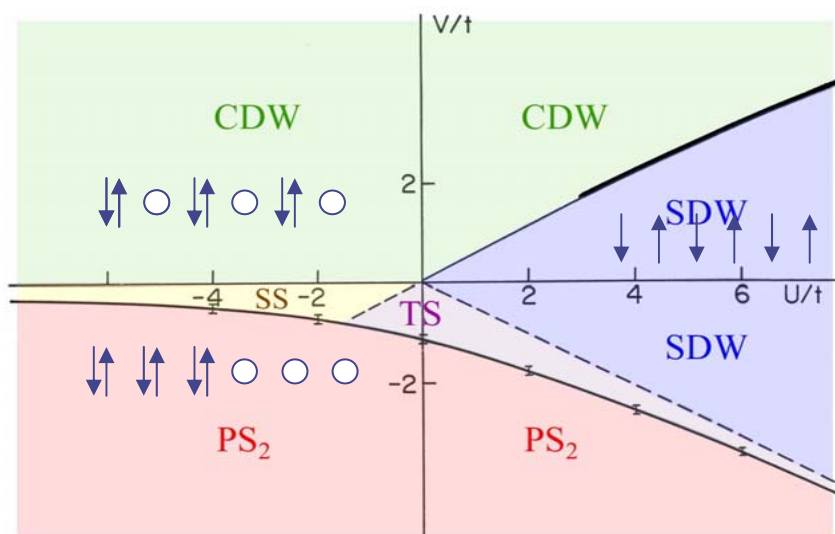
PRA, 68, 042330(2003).



Introduction: QPT & quantum entanglement

The extended
Hubbard model

$$H = - \sum_{\sigma,j,\delta} c_{j,\sigma}^+ c_{j+\delta,\sigma} + U \sum_j n_{j,\uparrow} n_{j,\downarrow} + V \sum_j n_j n_{j+1}$$



Phys. Rev. Lett. 93, 086402 (2004).

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Introduction: QPT & quantum entanglement

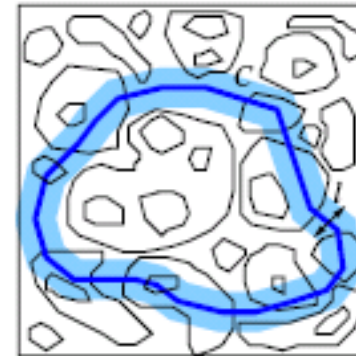
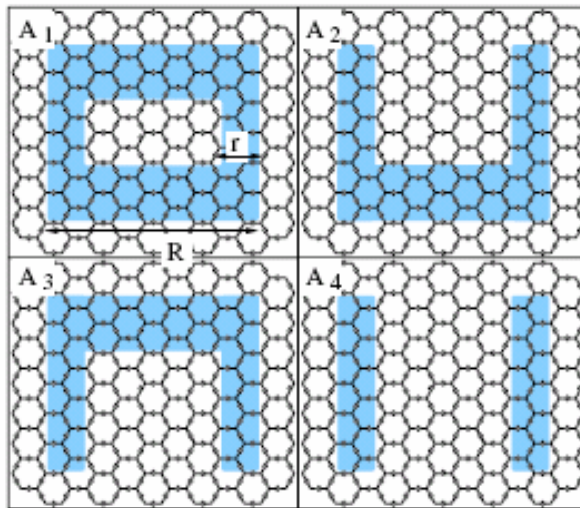
Detecting Topological Order in a Ground State Wave Function

Michael Levin and Xiao-Gang Wen

Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

(Received 25 October 2005; published 24 March 2006)

A large class of topological orders can be understood and classified using the string-net condensation picture. These topological orders can be characterized by a set of data $(N, d_i, F_{lmn}^{ijk}, \delta_{ijk})$. We describe a way to detect this kind of topological order using only the ground state wave function. The method involves computing a quantity called the “topological entropy” which directly measures the total quantum dimension $D = \sum_i d_i^2$.



$$(S_1 - S_2) - (S_3 - S_4)$$

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Introduction: QPT & Fidelity

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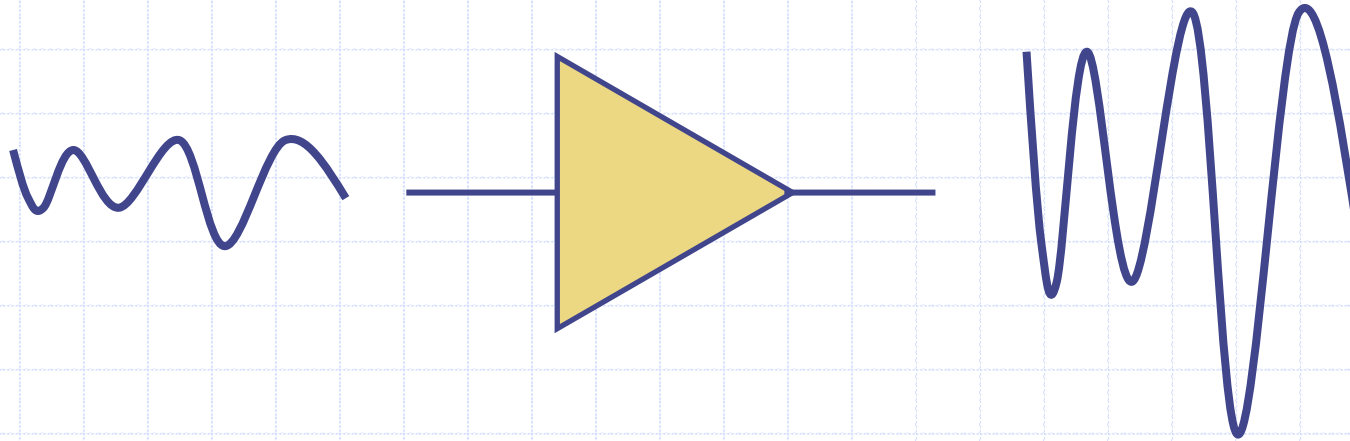


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Introduction: classical fidelity



Definition

$$\rho = p_1|1\rangle\langle 1| + p_2|2\rangle\langle 2| + \cdots + p_N|N\rangle\langle N|$$

$$\sigma = q_1|1\rangle\langle 1| + q_2|2\rangle\langle 2| + \cdots + q_N|N\rangle\langle N|$$

$$F = \sum_i \sqrt{p_i q_i}$$



Introduction: quantum fidelity

A. Uhlmann, Rep. Math. Phys. 9, 273 (1976)

$$F(\Psi', \Psi) = |\langle \Psi' | \Psi \rangle| \quad \mathbf{a} \cdot \mathbf{b} = ab \cos(\theta)$$

Axioms

R. Jozsa, J. Mod. Opt. 41, 2315 (1994).

$$0 \leq F(\Psi', \Psi) \leq 1,$$

$$F(\Psi', \Psi) = F(\Psi, \Psi'),$$

$$F(U\Psi', U\Psi) = F(\Psi', \Psi),$$

$$F(\Psi_1 \otimes \Psi_2, \Psi'_1 \otimes \Psi'_2) = F(\Psi'_1, \Psi_1)F(\Psi'_2, \Psi_2),$$

Example:

$$|\Psi(\theta)\rangle = \cos \theta |\uparrow\downarrow\rangle + \sin \theta |\downarrow\uparrow\rangle,$$

$$|\Psi(\theta')\rangle = \cos \theta' |\uparrow\downarrow\rangle + \sin \theta' |\downarrow\uparrow\rangle,$$

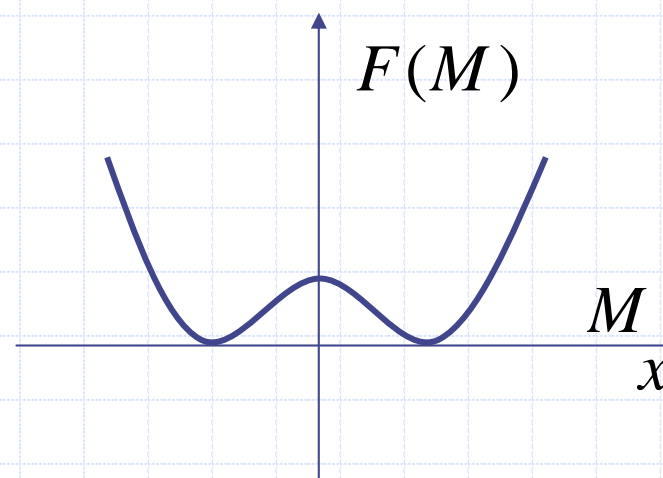
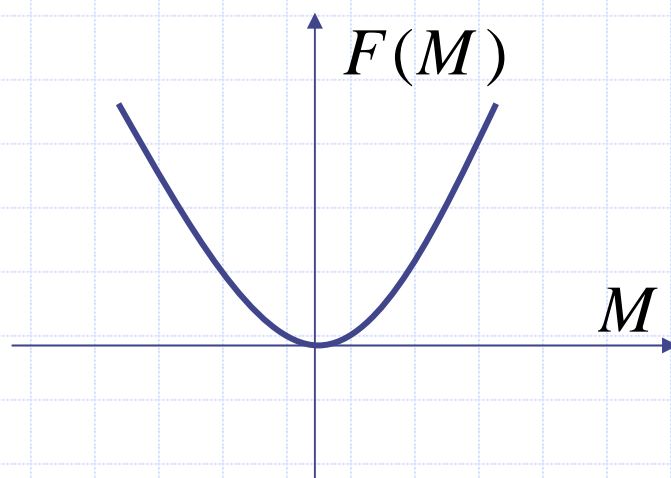
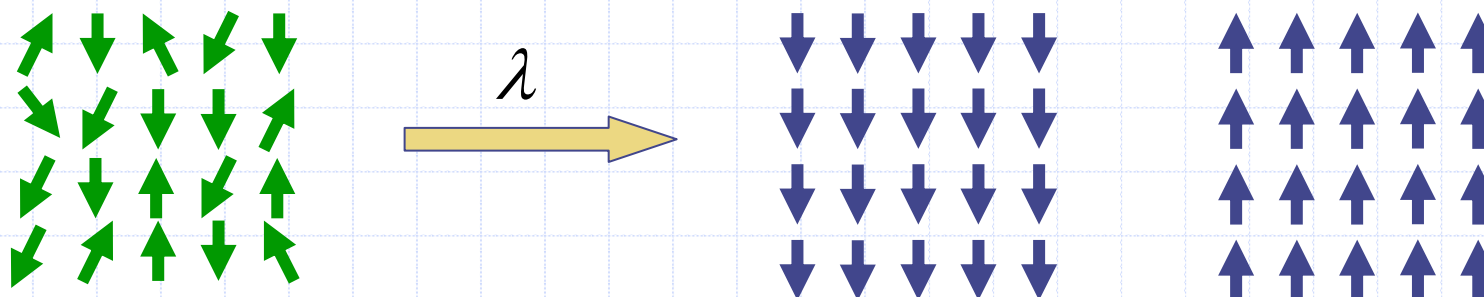
$$F(\Psi(\theta'), \Psi(\theta)) = |\cos(\theta - \theta')|.$$

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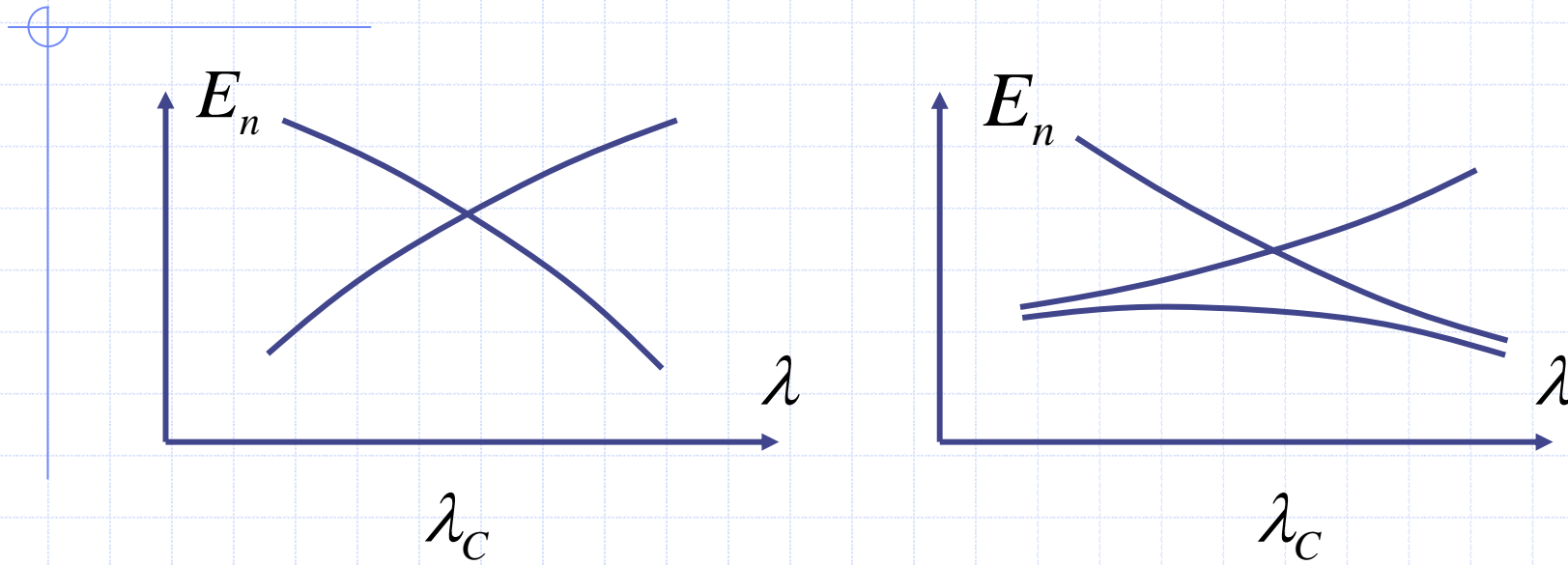
Introduction: traditional method

Landau's symmetry-breaking theory



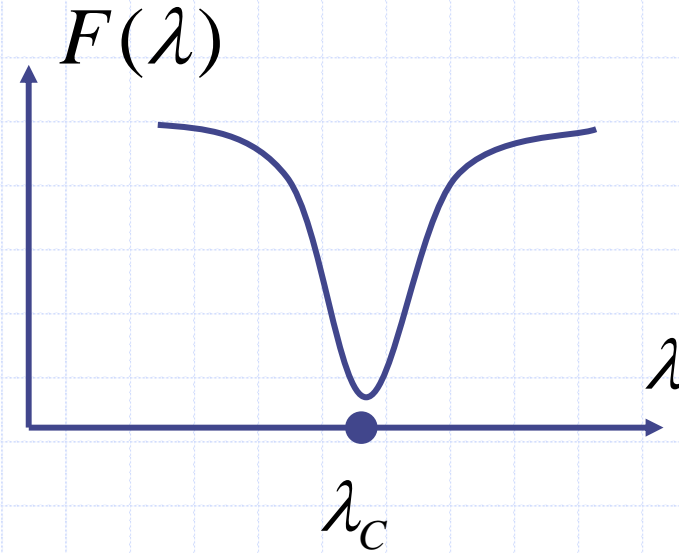
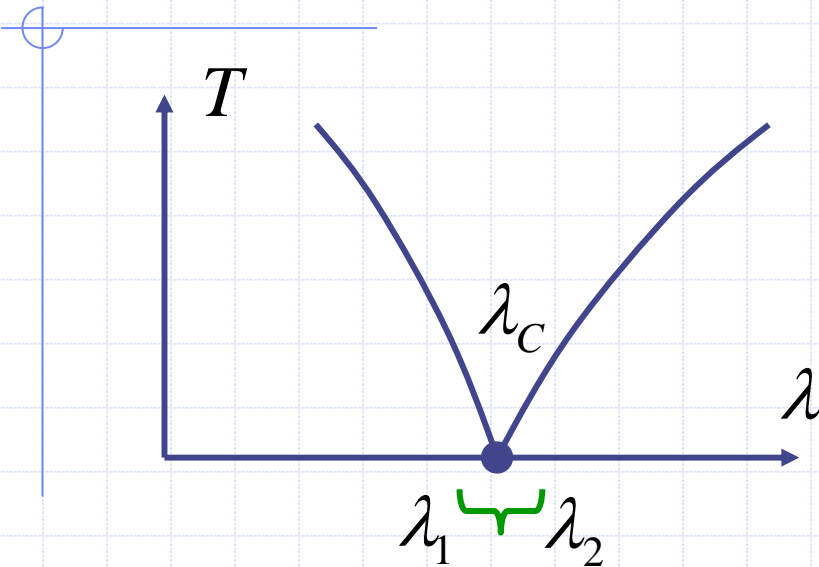


Introduction: information perspective





Introduction: information perspective



$$\psi(\lambda_1) \quad \psi(\lambda_2)$$

$$F = |\langle \psi(\lambda_1) | \psi(\lambda_2) \rangle|$$

$$\rho = \begin{pmatrix} a & \\ & b \end{pmatrix} \quad \sigma = \begin{pmatrix} c & \\ & d \end{pmatrix}$$

$$F(\rho, \sigma) = \sqrt{\rho^{1/2} \sigma \rho^{1/2}}$$

$$F(\rho, \sigma) = \sqrt{ac} + \sqrt{bd}$$



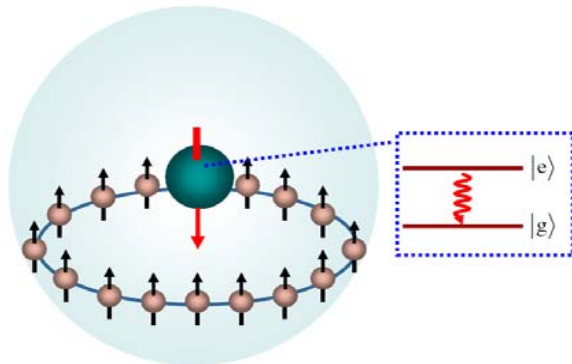
Introduction: QPT & Fidelity

Ising model

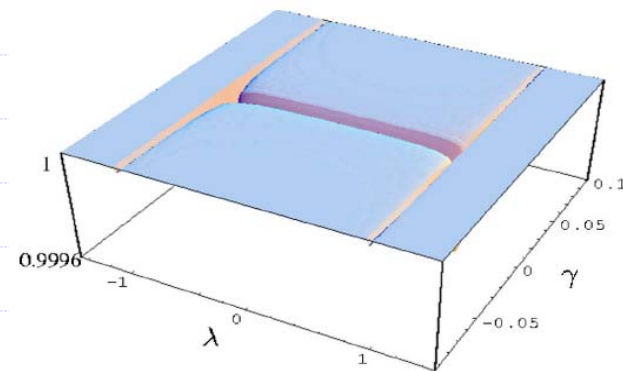
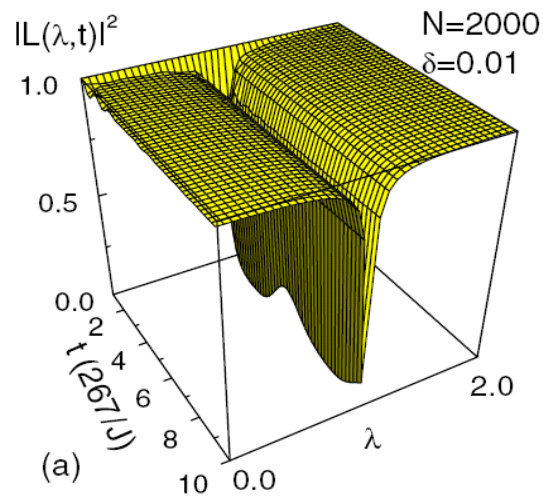
PRL **96**, 140604 (2006)

$$H(\lambda, \delta) = -J \sum_j (\sigma_j^z \sigma_{j+1}^z + \lambda \sigma_j^x + \delta |e\rangle\langle e| \sigma_j^x),$$

$$L(\lambda, t) = |\langle \varphi_g(t) | \varphi_e(t) \rangle|^2.$$



$$\hat{H}(\gamma, \lambda) = - \sum_{i=-M}^M \left(\frac{1+\gamma}{2} \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + \frac{1-\gamma}{2} \hat{\sigma}_i^y \hat{\sigma}_{i+1}^y + \frac{\lambda}{2} \hat{\sigma}_i^z \right).$$



PHYSICAL REVIEW E **74**, 031123 (2006)



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2. S. Chen, L. Wang, S. J. Gu, and Y. P. Wang, *Phys. Rev. E* **76**, 061108 (2007).
3. S. J. Gu, H. M. Kwok, W. Q. Ning, and H. Q. Lin, *Phys. Rev. B* **77**, 245109 (2008)
4. H. M. Kwok, W. Q. Ning, S. J. Gu, and H. Q. Lin, PRE accepted, arXiv: 0710.2581.
5. W. Q. Ning, S. J. Gu, C. Q. Wu, and H. Q. Lin, *J. Phys.: Condens. Matter* **20** 235236 (2008).
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Relevant works:

1. Partial-state fidelity and quantum phase transitions induced by continuous level crossing
Ho-Man Kwok, Chun-Sing Ho, and Shi-Jian Gu
2. Dimension of fidelity susceptibility in quantum phases
3. Scaling of reduced fidelity susceptibility in the one-dimensional transverse-field XY model
Wen-Long You, Wen-Long Lu, Xiaoguang Wang, and Shi-Jian Gu
4. Density-functional fidelity approach to quantum phase transitions,
Shi-Jian Gu, preprint.



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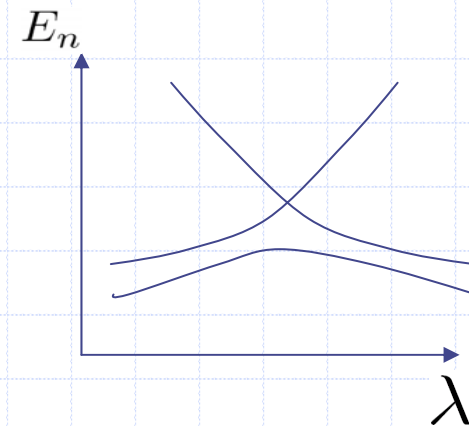
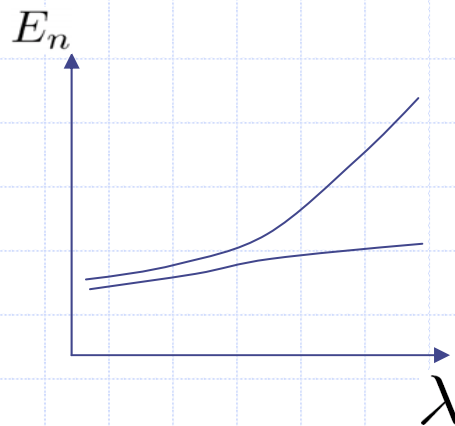
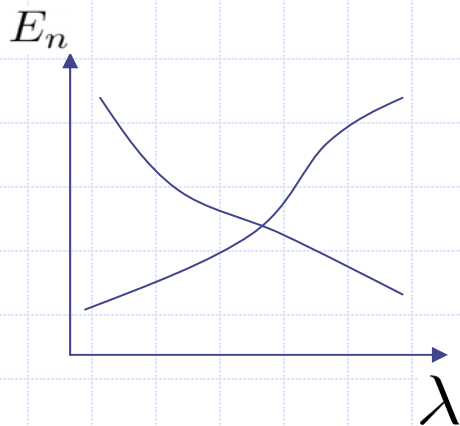


Occurrence of the quantum phase transitions

How does QPT happen for a general quantum system

$$H(\lambda) = H_0 + \lambda H_I,$$

$$H(\lambda)|\Psi_n(\lambda)\rangle = E_n|\Psi_n(\lambda)\rangle$$





Perturbation method in quantum mechanics

Fidelity susceptibility

$$|\Psi_0(\lambda + \delta\lambda)\rangle = |\Psi_0(\lambda)\rangle + \delta\lambda \sum_{n \neq 0} \frac{H_{n0}(\lambda) |\Psi_n(\lambda)\rangle}{E_0(\lambda) - E_n(\lambda)}$$

$$H_{n0} = \langle \Psi_n(\lambda) | H_I | \Psi_0(\lambda) \rangle.$$

$$F_i(\lambda, \delta) = |\langle \Psi_0(\lambda) | \Psi_0(\lambda + \delta) \rangle|$$

$$\frac{1}{F_i^2} = 1 + \delta\lambda^2 \sum_{n \neq 0} \frac{|\langle \Psi_n(\lambda) | H_I | \Psi_0(\lambda) \rangle|^2}{[E_n(\lambda) - E_0(\lambda)]^2}$$

$$\chi_F \equiv \lim_{\delta\lambda \rightarrow 0} \frac{-2 \ln F_i}{\delta\lambda^2} \quad \chi_F(\lambda) = \sum_{n \neq 0} \frac{|\langle \Psi_n(\lambda) | H_I | \Psi_0(\lambda) \rangle|^2}{[E_n(\lambda) - E_0(\lambda)]^2}$$



Perturbation method in quantum mechanics

Fidelity susceptibility: what is the physics

$$\chi_F(\omega) = \sum_{n \neq 0} \frac{|\langle \Psi_n | H_I | \Psi_0 \rangle|^2}{[E_n - E_0]^2 + \omega^2}$$

$$\begin{aligned} \frac{\partial \chi_F(\tau)}{\partial \tau} = & -\pi [\langle \Psi_0 | H_I(\tau) H_I(0) | \Psi_0 \rangle - \langle \Psi_0 | H_I | \Psi_0 \rangle^2] \theta(\tau) \\ & + \pi [\langle \Psi_0 | H_I(0) H_I(\tau) | \Psi_0 \rangle - \langle \Psi_0 | H_I | \Psi_0 \rangle^2] \theta(-\tau) \end{aligned}$$

Fidelity susceptibility = dynamic structure factor



Fidelity and dynamics structure factor

Fidelity susceptibility: how to compute

$$\chi_F = \int \tau [\langle \Psi_0 | H_I(\tau) H_I(0) | \Psi_0 \rangle - \langle \Psi_0 | H_I | \Psi_0 \rangle^2] d\tau$$

$$\begin{aligned} & \langle \Psi_0 | H_I(\tau) H_I(0) | \Psi_0 \rangle \\ &= \sum_n \frac{\tau^n (-1)^n}{n!} e^{\tau E_0} \langle \Psi_0 | H_I H^n H_I | \Psi_0 \rangle. \end{aligned}$$

To higher order

$$\chi_F = \frac{1}{H_I^{00}} \sum_{i,j>0} \frac{H_I^{0i} H_I^{ij} H_I^{j0}}{(E_i - E_0)(E_j - E_0)} - \frac{E_0^{(3)}}{E_0^{(1)}}.$$

S. Chen, L. Wang, Y. Hao, and Y. Wang, Phys. Rev. A 77, 032111 (2008).

L. C. Venuti, M. Cozzini, P. Buonsante, F. Massel, N. Bray-Ali, and P. Zanardi, arXiv:0801.2473.

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Extension to thermal phase transitions

Fidelity susceptibility: extension to TPT

P. Zanardi, H. T. Quan, X. Wang, and C. P. Sun, Phys. Rev. A
75, 032109 (2007).

$$F_i(\beta, \delta) = \frac{Z(\beta)}{\sqrt{Z(\beta - \delta\beta/2)Z(\beta + \delta\beta/2)}},$$

$$Z(\beta) = \sum_n e^{-\beta E_n} = \sum_E g(E) e^{-\beta E}.$$

You, Li, and Gu, PRE, 76, 022101 (2007)

$$\chi_F = \left. \frac{-2 \ln F_i}{\delta\beta^2} \right|_{\delta\beta \rightarrow 0} = \frac{C_v}{4\beta^2} \quad C_v = \beta^2 (\langle E^2 \rangle - \langle E \rangle^2)$$

$$\chi_F = \left. \frac{-2 \ln F_i}{\delta h^2} \right|_{\delta h \rightarrow 0} = \frac{\beta\chi}{4} \quad \chi = \beta (\langle \dot{M}^2 \rangle - \langle \dot{M} \rangle^2)$$

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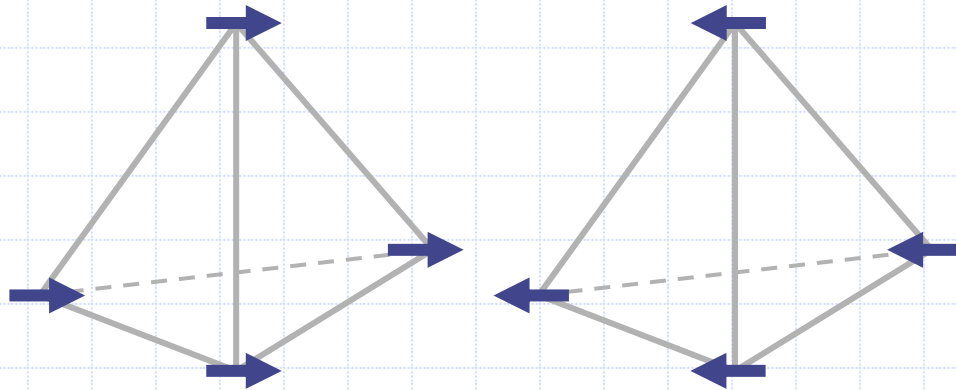
Application: the Lipkin-Meshkov-Glick model

Hamiltonian

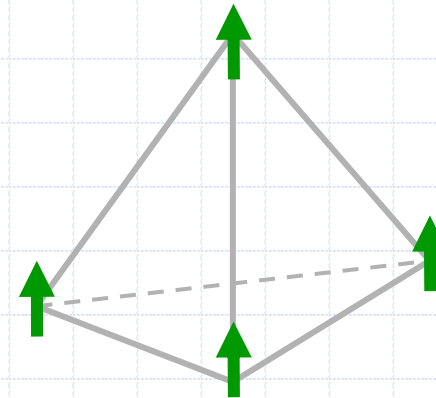
$$H = -\frac{\lambda}{N} \sum_{i < j} (\sigma_x^i \sigma_x^j + \gamma \sigma_y^i \sigma_y^j) - h \sum_i \sigma_z^i,$$

Ground phases (ferromagnetic)

$h < 1$



$h > 1$





Application: the LMG model

If $h > 1$

$$\begin{aligned}S_z &= S - a^\dagger a, \\S_+ &= (2S - a^\dagger a)^{1/2} a\end{aligned}$$

The Hamiltonian in terms of bosons

$$H = -hN + [2(h - 1) + \eta]a^\dagger a - \frac{\eta}{2} (a^{\dagger 2} + a^2)$$

$$\begin{aligned}a^\dagger &= \cosh(\Theta/2)b^\dagger + \sinh(\Theta/2)b, \\a &= \sinh(\Theta/2)b^\dagger + \cosh(\Theta/2)b,\end{aligned}$$

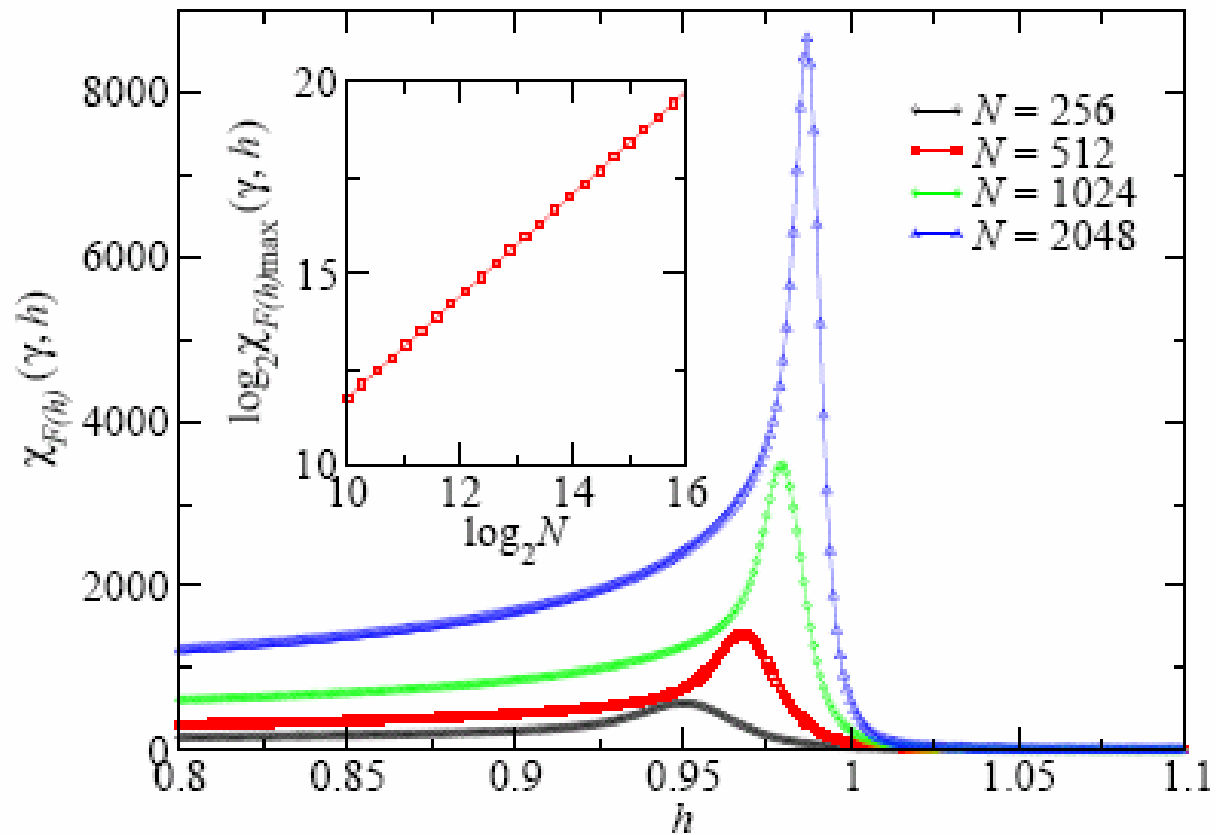
The diagonalized form

$$H = -h(N + 1) + 2 \sqrt{(h - 1)(h - 1 + \eta)} \left(b^\dagger b + \frac{1}{2} \right)$$



Application: the LMG model

$$\gamma = 0.5$$





Universality class described by the FS

The fidelity susceptibility

L. C. Venuti and P. Zanardi, Phys. Rev. Lett. **99**, 095701 (2007).

$$\chi_F = \int \tau [\langle \Psi_0 | H_I(\tau) H_I(0) | \Psi_0 \rangle - \langle \Psi_0 | H_I | \Psi_0 \rangle^2] d\tau$$

$$r' = s r, \quad \tau' = s^\zeta \tau, \quad V(r') = s^{-\Delta_V} V(r)$$

$$\chi_F \sim L^{2\Delta_V - 2\zeta}$$

S. J. Gu, H. M. Kwok, W. Q. Ning, and H. Q. Lin, Phys. Rev. B **77**, 245109 (2008).

$$\frac{\chi_{F(\lambda)}(\lambda)}{N} \propto \frac{1}{|\lambda_c - \lambda|^\alpha} \quad N = L^d$$



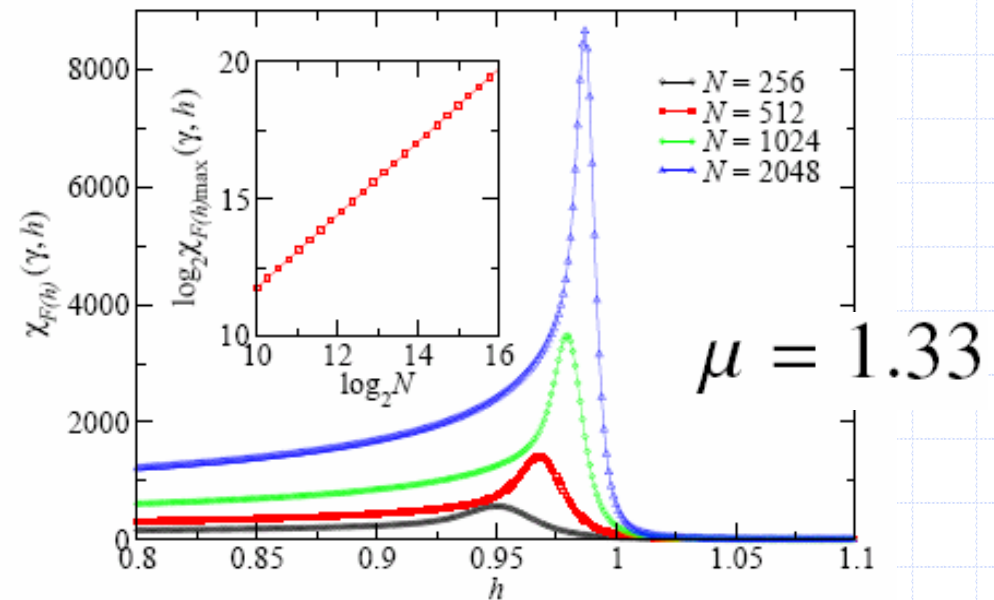
Application: asymmetric Hubbard model

Scaling ansatz: d (adiabatic dimension)

$$\frac{\chi(\lambda, L)}{L^{d^\pm}} = \frac{A}{L^{-\mu+d^\pm} + B(\lambda - \lambda_{\max})^\alpha}$$

$$\chi(\lambda = \lambda_{\max}) \propto L^\mu$$

$$\frac{\chi_F}{L^{d_a^\pm}} \sim \frac{1}{|\lambda - \lambda_c|^\alpha}$$





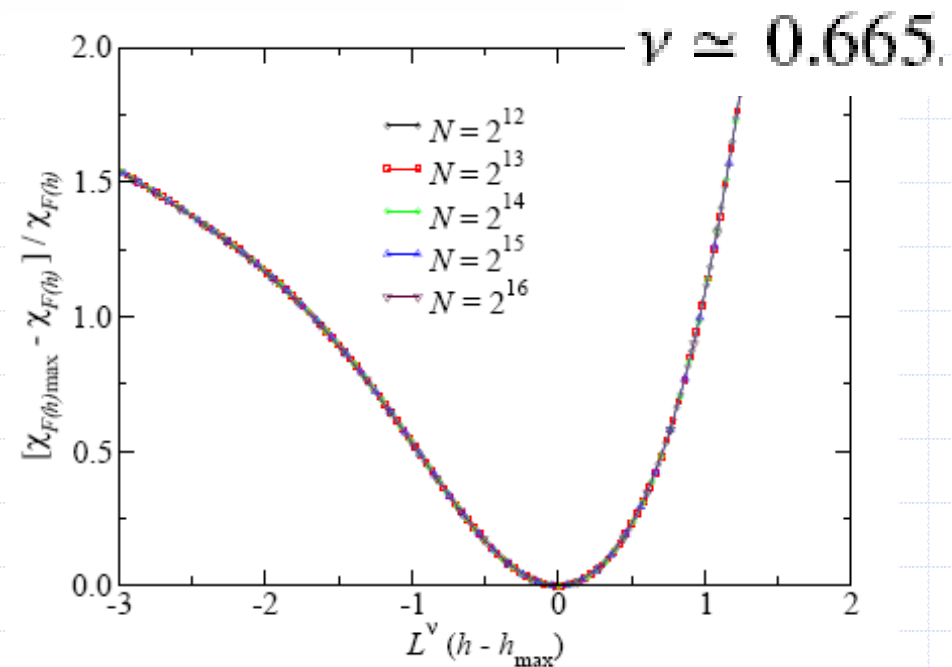
Application: asymmetric Hubbard model

Universal function

$$\frac{\chi_{F(\lambda)}(\lambda = \lambda_{\max}, L) - \chi_{F(\lambda)}(\lambda, L)}{\chi_{F(\lambda)}(\lambda, L)} = f[L^\nu(\lambda - \lambda_{\max})]$$

Critical exponent

$$\alpha^\pm = \frac{\mu - d^\pm}{\nu}$$
$$\alpha = \begin{cases} 2, & h > 1 \\ \frac{1}{2}, & 0 \leq h < 1 \end{cases}$$





Application: the LMG model

If $h > 1$

$$-\sum_i \sigma_z^i = -2S_z$$

$$\chi_{F(h)}(\eta, h > 1) = \frac{\eta^2}{32(h-1)^2(h-1+\eta)^2}$$

If $h < 1$

$$\frac{\chi_{F(h)}(\eta, h < 1)}{N} = \frac{1}{4\sqrt{(1-h^2)\eta}}$$

Exponents

$$\alpha = \begin{cases} 2, & h > 1 \\ \frac{1}{2}, & 0 \leq h < 1 \end{cases}$$

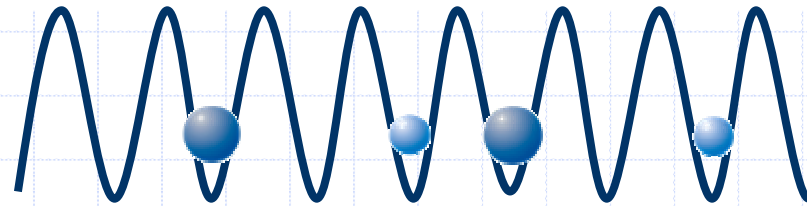


Application: asymmetric Hubbard model

$$H = - \sum_{j=1}^L \sum_{\delta=\pm 1} \sum_{\sigma} t_{\sigma} c_{j,\sigma}^{\dagger} c_{j+\delta,\sigma} + U \sum_{j=1}^L n_{j,\alpha} n_{j,\beta}.$$

$$\sigma = \alpha, \beta$$

$$t_{\alpha} = 1, t_{\beta} \in [0, 1]$$



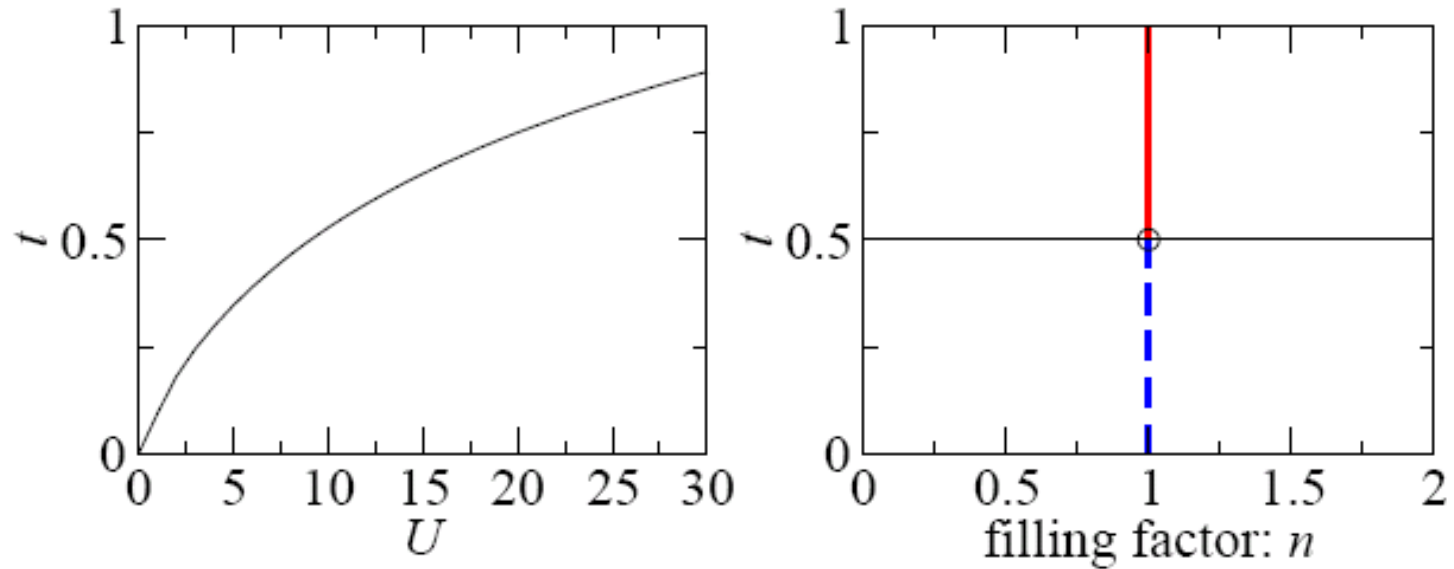
$$V_0 = v \frac{\hbar^2 k^2}{2m},$$

$$\frac{t_{\beta}}{t_{\alpha}} = \frac{m_{\alpha}}{m_{\beta}},$$

$$\frac{U}{t_{\alpha}} = \frac{16a \sqrt{\pi m_{\alpha}/m_{\beta}}}{\lambda} \frac{v^{1/4} v_{\perp}^{1/2}}{(\sqrt{v} + 2\sqrt{v_{\perp}})} e^{\pi^2 \sqrt{v}}$$



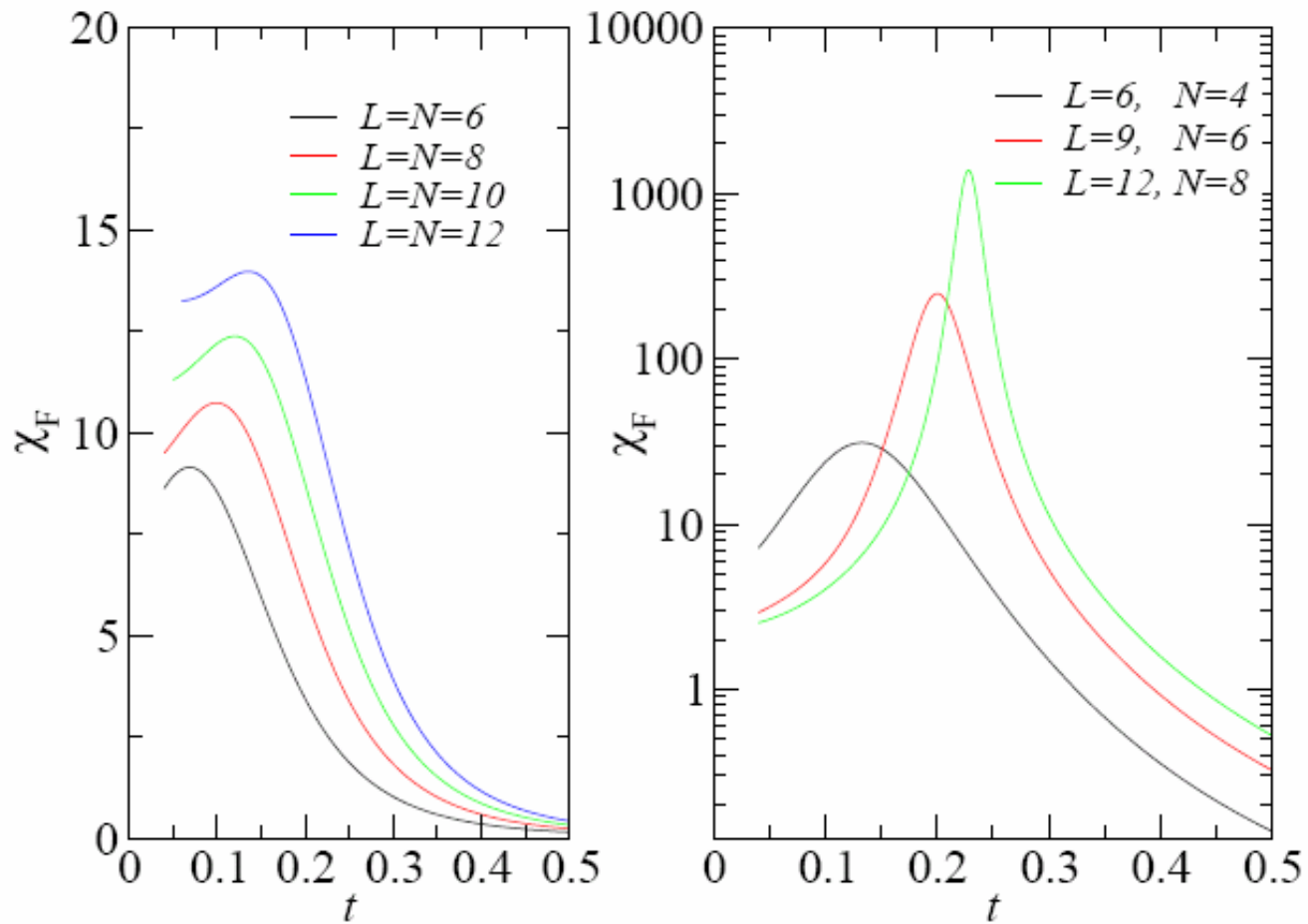
Application: asymmetric Hubbard model



The schematic phase diagram of the asymmetric Hubbard model



Application: asymmetric Hubbard model





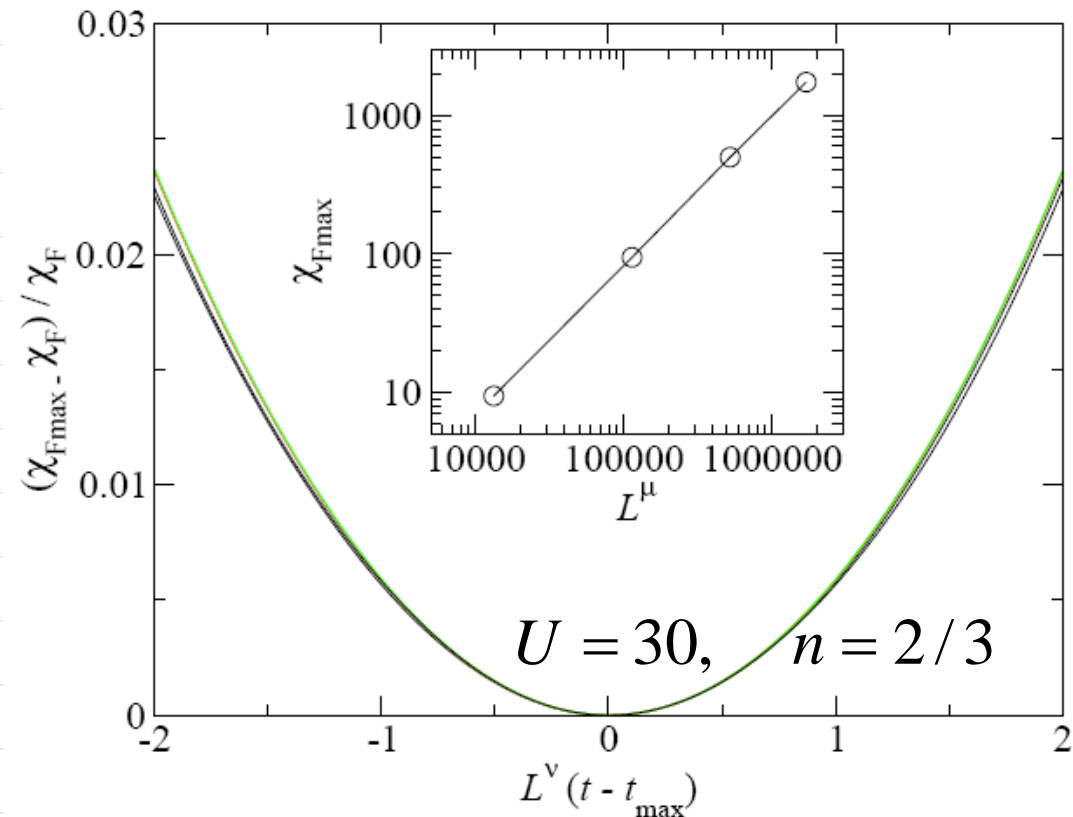
Application: asymmetric Hubbard model

$$\frac{\chi_{F(t)}(t = t_{\max}) - \chi_{F(t)}(t)}{\chi_{F(t)}(t)} = g[L^\nu(t - t_{\max})]$$

$$\mu = 5.3,$$

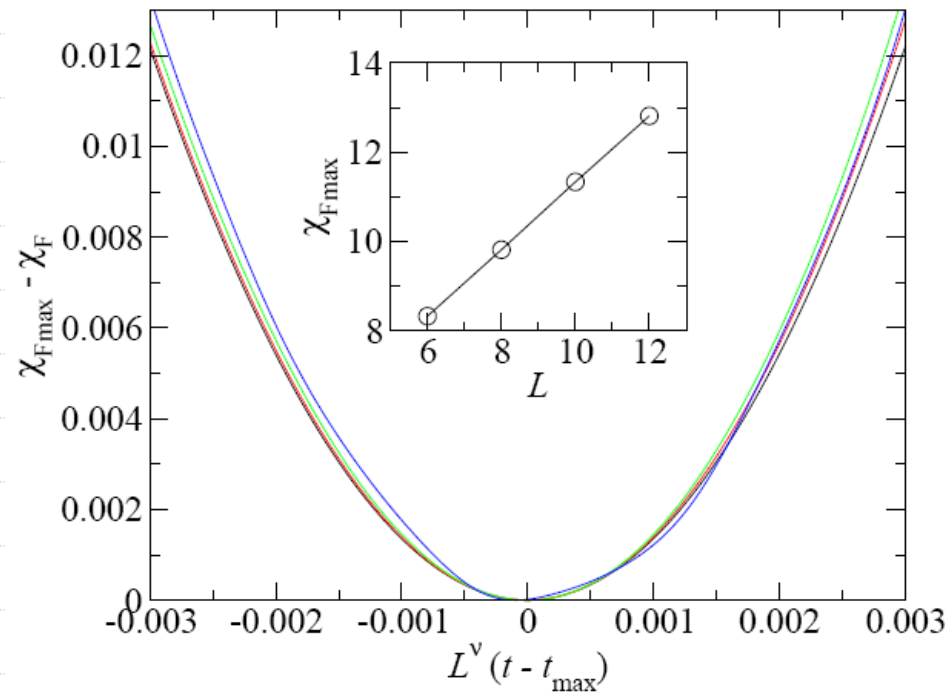
$$\nu = 2.65$$

$$\alpha = (\mu - 1) / \nu \\ = 0.6$$





Application: asymmetric Hubbard model



$$U = 30, \quad n = 1$$

$$\chi_F(t)(t) \simeq 3.855 + 0.7478L + 1349.9L^{-1/2}(t - t_{\max})^2$$



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- VI. Summary**

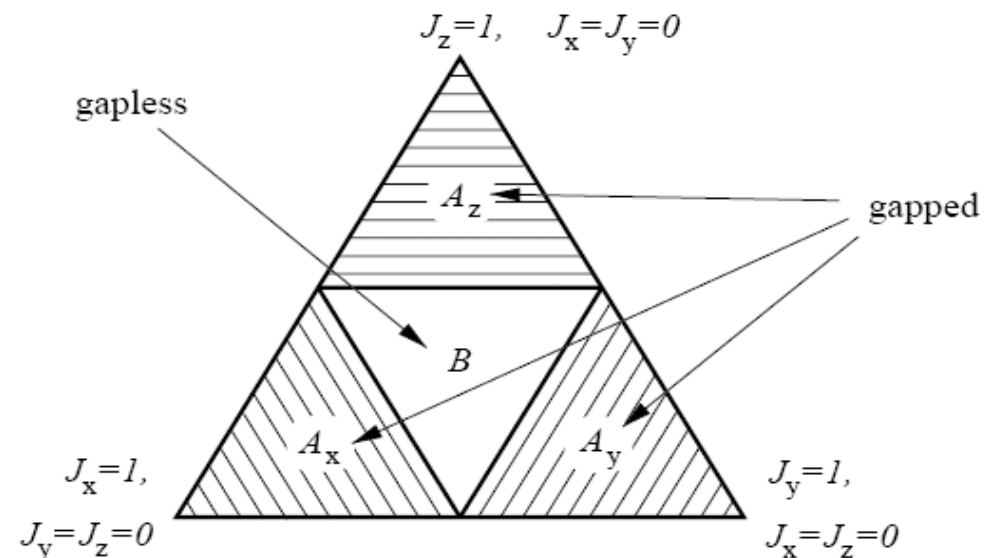
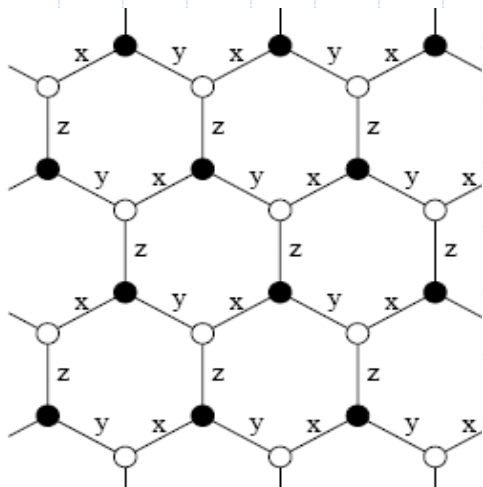


The Kitaev honeycomb model

A. Kitaev, Ann. Phys. **303**, 2 (2003); Ann. Phys. **321**, 2 (2006).

$$H = -J_x \sum_{x\text{-bonds}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-bonds}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-bonds}} \sigma_j^z \sigma_k^z,$$

$$J_x + J_y + J_z = 1$$



X. G. Wen, *Quantum Field Theory of Many-Body Systems* (Oxford University, New York, 2004).



The critical fidelity susceptibility

$$\sigma^x = ib^x c, \quad \sigma^y = ib^y c, \quad \sigma^z = ib^z c.$$

$$H = \frac{i}{2} \sum_{j,k} \hat{u}_{jk} J_{a_{jk}} c_j c_k$$

$$H = \sum_{\mathbf{q}} \begin{pmatrix} a_{-\mathbf{q},1} \\ a_{-\mathbf{q},2} \end{pmatrix}^T \begin{pmatrix} 0 & if(\mathbf{q}) \\ -if(\mathbf{q})^* & 0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{q},1} \\ a_{\mathbf{q},2} \end{pmatrix}$$

$$H = \sum_{\mathbf{q}} \sqrt{\epsilon_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2} \left(C_{\mathbf{q},1}^\dagger C_{\mathbf{q},1} - C_{\mathbf{q},2}^\dagger C_{\mathbf{q},2} \right)$$

$$f(\mathbf{q}) = \epsilon_{\mathbf{q}} + i\Delta_{\mathbf{q}},$$

$$\epsilon_{\mathbf{q}} = J_x \cos q_x + J_y \cos q_y + J_z$$

$$\Delta_{\mathbf{q}} = J_x \sin q_x + J_y \sin q_y.$$



The critical fidelity susceptibility

$$\begin{aligned} |\Psi_0\rangle &= \prod_{\mathbf{q}} C_{\mathbf{q},2}^\dagger |0\rangle \\ &= \prod_{\mathbf{q}} \frac{1}{\sqrt{2}} \left(\frac{\sqrt{\epsilon_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2}}{\Delta_{\mathbf{q}} + i\epsilon_{\mathbf{q}}} a_{-\mathbf{q},1} + a_{-\mathbf{q},2} \right) |0\rangle \end{aligned}$$

$$E_0 = - \sum_{\mathbf{q}} \sqrt{\epsilon_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2}.$$

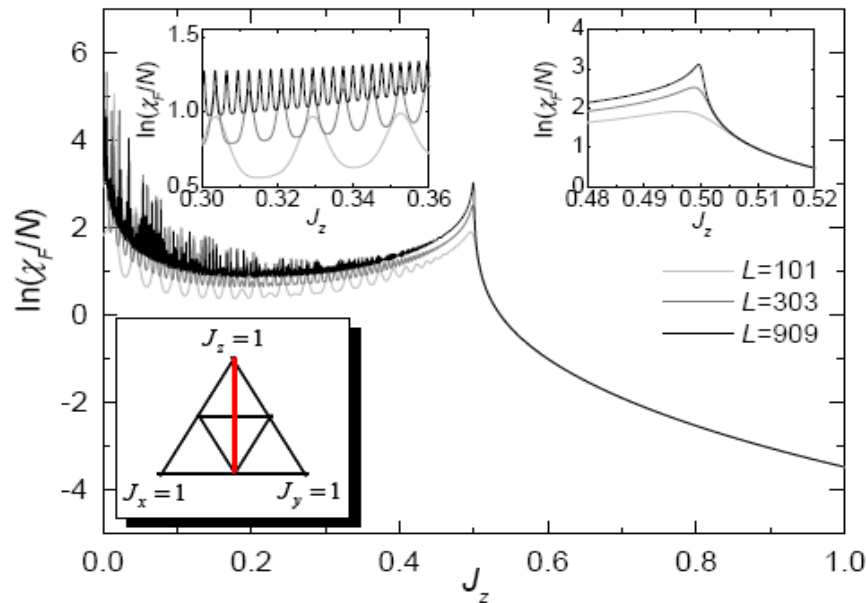
$$F^2 = \prod_{\mathbf{q}} \frac{1}{2} \left(1 + \frac{\Delta_{\mathbf{q}} \Delta'_{\mathbf{q}} + \epsilon_{\mathbf{q}} \epsilon'_{\mathbf{q}}}{E_{\mathbf{q}} E'_{\mathbf{q}}} \right)$$

$$\chi_F \equiv \lim_{\delta\lambda \rightarrow 0} \frac{-2 \ln F_i}{\delta\lambda^2}$$

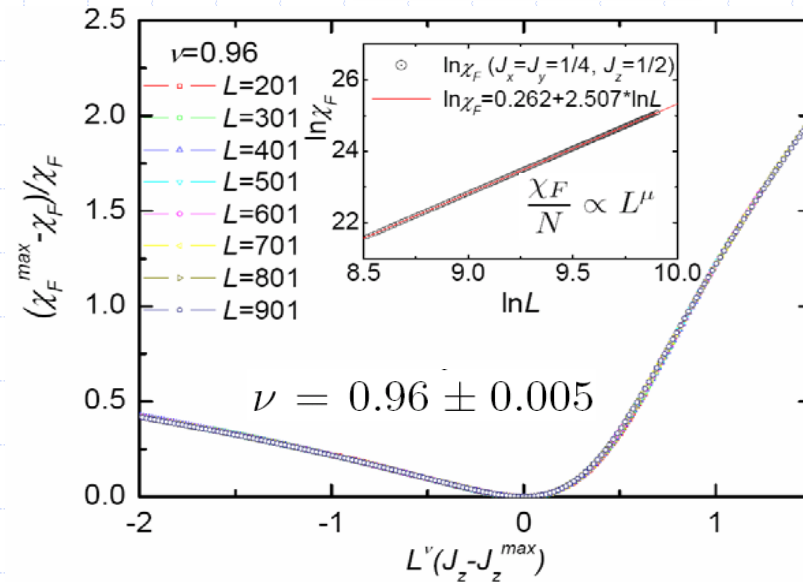


The critical fidelity susceptibility

$$\chi_F = \frac{1}{16} \sum_{\mathbf{q}} \left[\frac{\sin q_x + \sin q_y}{\epsilon_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2} \right]^2$$



$$\mu = 0.507 \pm 0.0001$$



$$\frac{\chi_F^{\max} - \chi_F}{\chi_F} = f[L^\nu (J_z - J_z^{\max})]$$

$$\frac{\chi_F}{N} \propto \frac{1}{|J_z - J_z^c|^\alpha} \quad \alpha = \frac{\mu}{\nu} = 0.528 \pm 0.001$$



The first conclusion on topological phase transition

- **The fidelity susceptibility can be used to witness the topological quantum phase transition in the Kitaev model**

Title: Singularity in ground state fidelity and quantum phase transitions for the Kitaev model

Authors: [Jian-Sheng Chen](#), [Huan-Qiang Zhou](#), [arXiv:0803.0814](#)

Title: Scaling of fidelity susceptibility at the ground state of Kitaev honeycomb model

Authors: [Shuo Yang](#), [Shi-Jian Shao](#), [Chang-Pu Sun](#), [Hai-Qing Lin](#), [arXiv:0803.1292](#)

Fidelity analysis of topological quantum phase transitions

Authors: [Damian F. Abasto](#), [Alicia Hamma](#), [Paolo Zanardi](#), [arXiv:0803.2243](#)



The bond-bond correlation

Fidelity susceptibility W. L. You, Y. W. Li, and S. J. Gu, Phys. Rev. E **76**, 022101 (2007).

$$\chi_F = \int \tau [\langle \Psi_0 | H_I(\tau) H_I(0) | \Psi_0 \rangle - \langle \Psi_0 | H_I | \Psi_0 \rangle^2] d\tau$$

Bond-bond correlation function

$$C(\mathbf{r}_1, \mathbf{r}_2) = \langle \sigma_{\mathbf{r}_1,1}^z \sigma_{\mathbf{r}_1,2}^z \sigma_{\mathbf{r}_2,1}^z \sigma_{\mathbf{r}_2,2}^z \rangle - \langle \sigma_{\mathbf{r}_1,1}^z \sigma_{\mathbf{r}_1,2}^z \rangle \langle \sigma_{\mathbf{r}_2,1}^z \sigma_{\mathbf{r}_2,2}^z \rangle$$



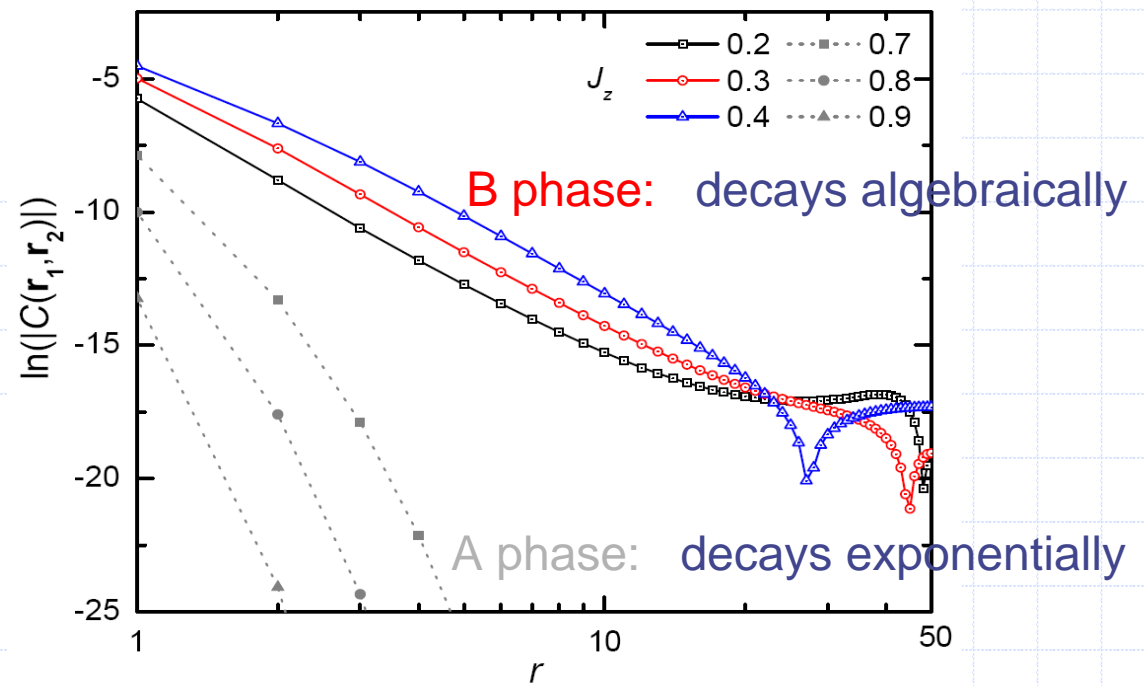
The bond-bond correlation

$$\langle \sigma_{\mathbf{r}_{1,1}}^z \sigma_{\mathbf{r}_{1,2}}^z \rangle = \langle \sigma_{\mathbf{r}_{2,1}}^z \sigma_{\mathbf{r}_{2,2}}^z \rangle = \frac{1}{N} \sum_{\mathbf{q}} \frac{\epsilon_{\mathbf{q}}}{E_{\mathbf{q}}}$$

$$\begin{aligned} & \langle \Psi_0 | \sigma_{\mathbf{r}_{1,1}}^z \sigma_{\mathbf{r}_{1,2}}^z \sigma_{\mathbf{r}_{2,1}}^z \sigma_{\mathbf{r}_{2,2}}^z | \Psi_0 \rangle \\ &= \frac{1}{N^2} \sum_{\mathbf{q}, \mathbf{q}'} \{ \cos [(\mathbf{q} - \mathbf{q}') (\mathbf{r}_1 - \mathbf{r}_2)] - 1 \} \\ & \quad \times \frac{(\Delta_{\mathbf{q}} \Delta_{\mathbf{q}'} - \epsilon_{\mathbf{q}} \epsilon_{\mathbf{q}'})}{E_{\mathbf{q}} E_{\mathbf{q}'}} \end{aligned}$$

$$C(\mathbf{r}_1, \mathbf{r}_2) \propto \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|^4}$$

$$\frac{1}{\xi} = 2 \sinh^{-1} \frac{\sqrt{2J_z - 1}}{1 - J_z}$$





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Beyond the pure-state fidelity

1. Fidelity per site H. Q. Zhou, J. H. Zhao, and B. Li, arXiv:0704.2940;
2. Operator fidelity X. Wang, Z. Sun, and Z. D. Wang, arXiv:0803.2940
3. Density-functional fidelity (SJGu, preprint)
4. Reduced fidelity (Zhou. Peres. Wang. GU)



The density-functional theory

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_I + \sum_x \mu_x \hat{n}_x$$

the density-functional fidelity (DFF). According to the Hohenberg-Kohn theorems, the ground-state properties of a quantum many-body system is uniquely determined by the density distribution n_x that minimize the functional for the ground-state energy $E_0[n_x]$. Therefore, the distribution n_x captures the most relevant information about the ground-state. Any change in the structure of the wavefunction can be found by calculating the similarity between two density distributions, i.e. the fidelity,



The density-functional fidelity

$$\rho(x_1, x'_1) = \text{tr} |\Psi_0(\lambda)\rangle \langle \Psi_0(\lambda)|$$

$$n = \sum_x n_x |x\rangle \langle x|$$

$$n_x = \langle \Psi_0(\lambda) | \hat{n}_x | \Psi_0(\lambda) \rangle = \langle \Psi_0(\lambda) | (\partial \hat{H} / \partial \mu_x) | \Psi_0(\lambda) \rangle$$

$$F(\lambda, \lambda') = \text{tr} \sqrt{n(\lambda) n(\lambda')}$$



The density-functional theory

$$F(\lambda, \lambda') = \text{tr} \sqrt{n(\lambda)n(\lambda')}$$

$$F(\lambda, \lambda + \delta\lambda) = 1 - \frac{(\delta\lambda)^2}{2} \chi_F.$$

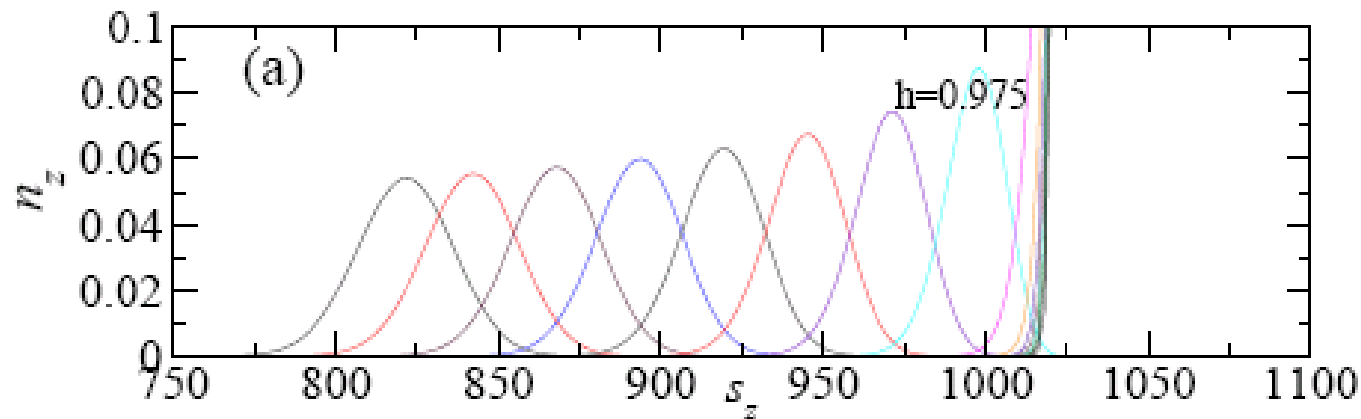
$$\chi_F = \sum_x \frac{1}{4n_x} \left(\frac{\partial n_x}{\partial \lambda} \right)^2$$



Example: the LMG model

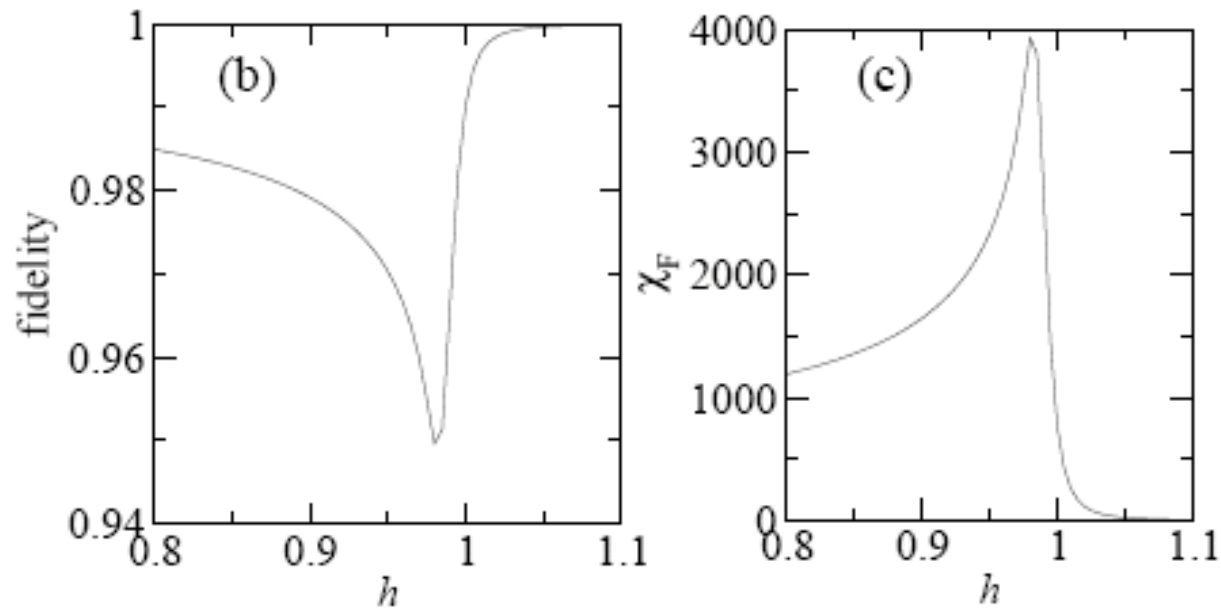
$$H = -\frac{\lambda}{2S} (1 + \gamma) (\hat{\mathbf{S}}^2 - \hat{S}_z^2 - S) - 2h\hat{S}_z - \frac{\lambda}{4S} (1 - \gamma) (\hat{S}_+^2 + \hat{S}_-^2),$$

$$|\Psi_0(h)\rangle = \sum \varphi(s_z) |s_z\rangle \quad n_z = \langle \Psi_0(h) | \hat{S}_z | \Psi_0(h) \rangle$$





Example: the LMG model



For the LMG model, the density-functional fidelity is the same as the pure-state fidelity because the LMG model become a single-particle problem in the anisotropic case.



Example: Hubbard model

$$H = -\sum_{\sigma, j} (c_{j, \sigma}^+ c_{j+1, \sigma} + c_{j+1, \sigma}^+ c_{j, \sigma}) + U \sum_j n_{j, \uparrow} n_{j, \downarrow}$$

$$2\pi I_j = k_j L - 2 \sum_{a=1}^M \tan^{-1} \left(\frac{\lambda_a - \sin k_j}{U/4} \right)$$

$$2\pi J_a = 2 \sum_{j=1}^N \tan^{-1} \left(\frac{\lambda_a - \sin k_j}{U/4} \right) - 2 \sum_{b=1}^M \tan^{-1} \left(\frac{\lambda_a - \lambda_b}{U/2} \right)$$

$$E = -2 \sum_{j=1}^N \cos k_j$$

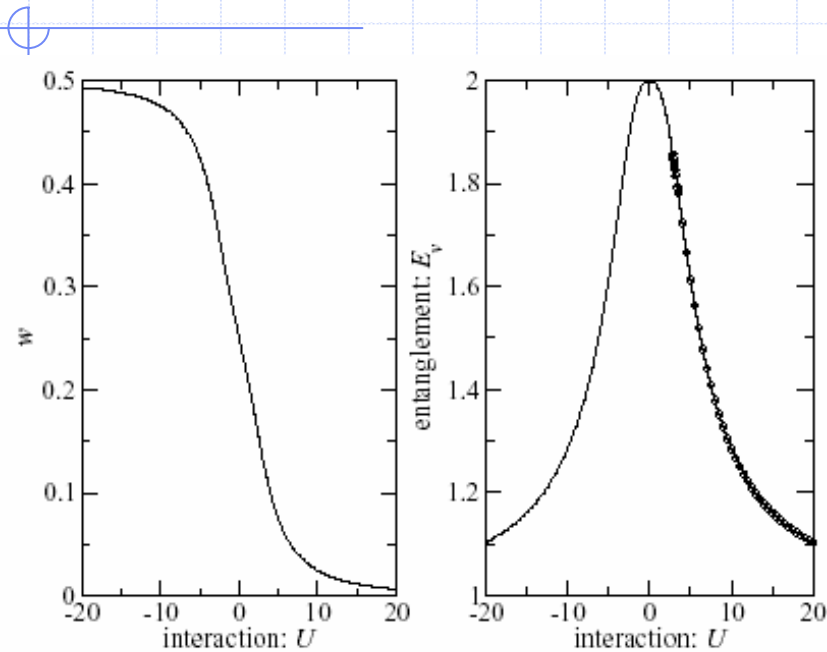
$$I_j = -\frac{N-1}{2}, -\frac{N-3}{2}, \dots, \frac{N-1}{2}$$

$$J_a = -\frac{M-1}{2}, -\frac{M-3}{2}, \dots, \frac{M-1}{2}$$

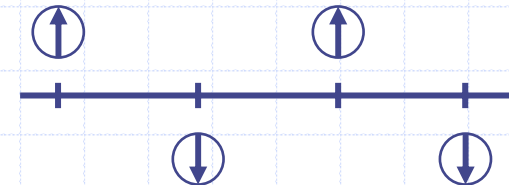
Hellman-Feynman定理: $w = \frac{1}{N} \frac{dE(U)}{dU}$



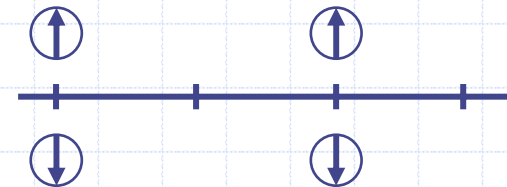
Example: Hubbard model



$U > 0$



$U < 0$



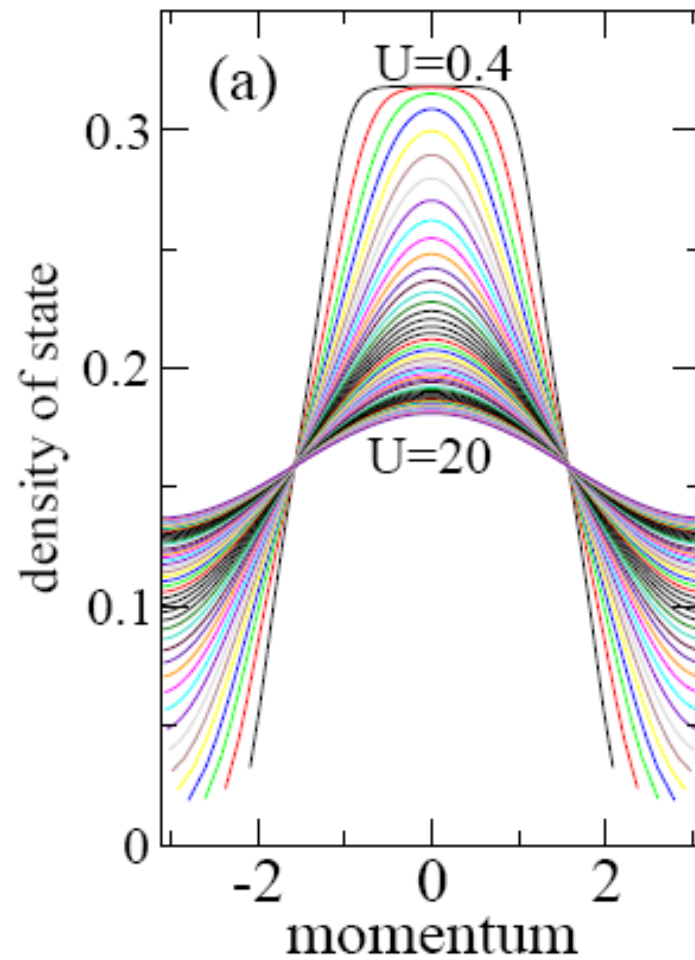
$$E_v(U) = E_v(-U)$$

$$w = \int_0^\infty \frac{J_0(\omega)J_1(\omega)d\omega}{1 + \cosh(U\omega/2)}$$

$$E_v = -2w \log_2 w - 2(1/2 - w) \log_2(1/2 - w)$$

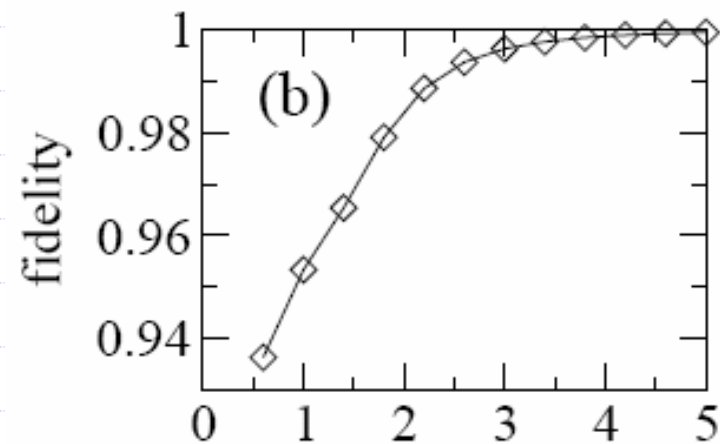


Example: Hubbard model



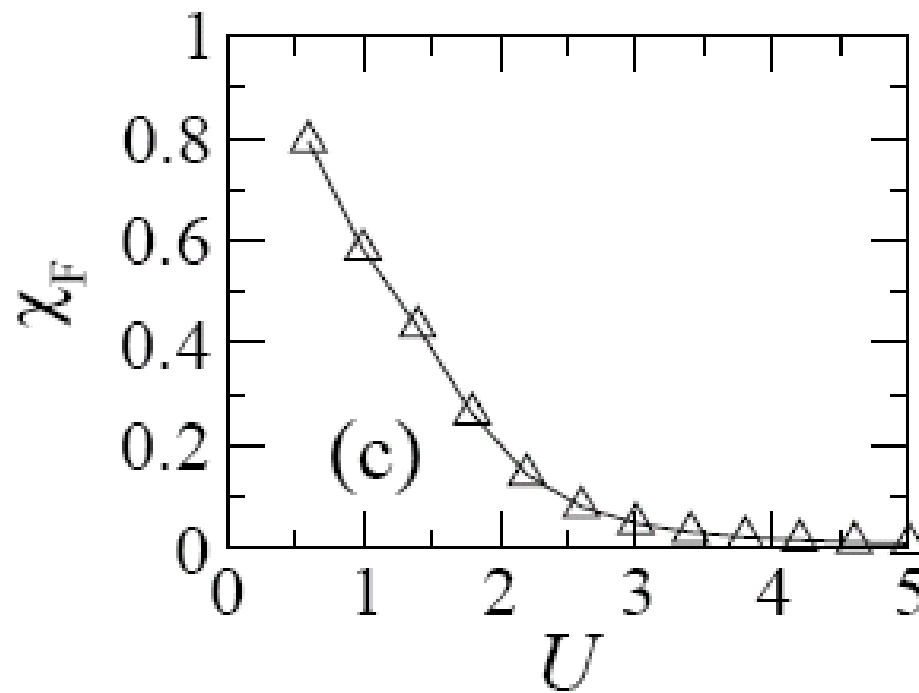
$$\rho\left(\frac{k_j + k_{j+1}}{2}\right) = \frac{1}{L(k_{j+1} + k_j)}$$

$$\frac{N}{L} = \int \rho(k) dk$$





Example: Hubbard model

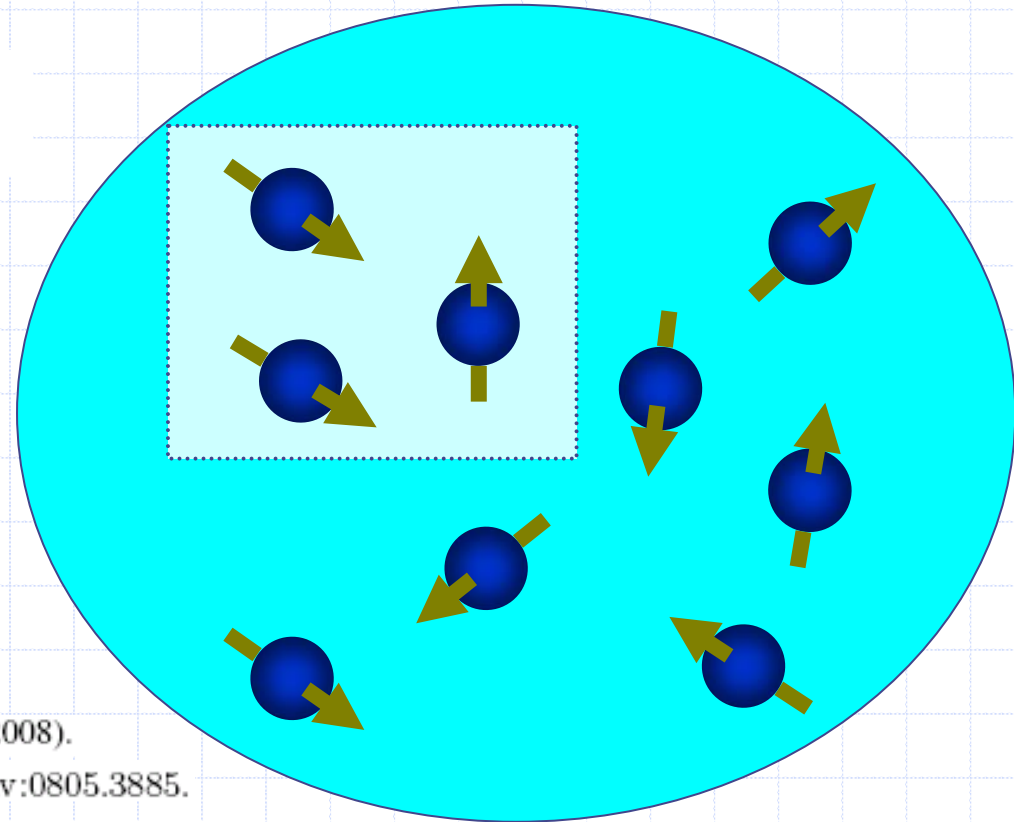




Example: Reduced fidelity

$$F_A(h, \bar{h}) = \text{Tr} \sqrt{\sqrt{\hat{\rho}_A(h)} \hat{\rho}_A(\bar{h}) \sqrt{\hat{\rho}_A(h)}}.$$

$$\rho_A(\bar{h}) = \frac{1}{2} \begin{pmatrix} 1 + \langle \sigma^z \rangle & 0 \\ 0 & 1 - \langle \sigma^z \rangle \end{pmatrix}.$$



H. Q. Zhou, arXiv:0704.2945.

N. Paunkovic *et al*, Phys. Rev. A **77**, 052302 (2008).

H. M. Kwok, C. S. Ho, and S. J. Gu, arXiv:0805.3885.

J. Ma, L. Xu, H. Xiong, and X. Wang, arXiv:0805.4062.

J. Ma, L. Xu, and X. Wang, arXiv:0808.1816.

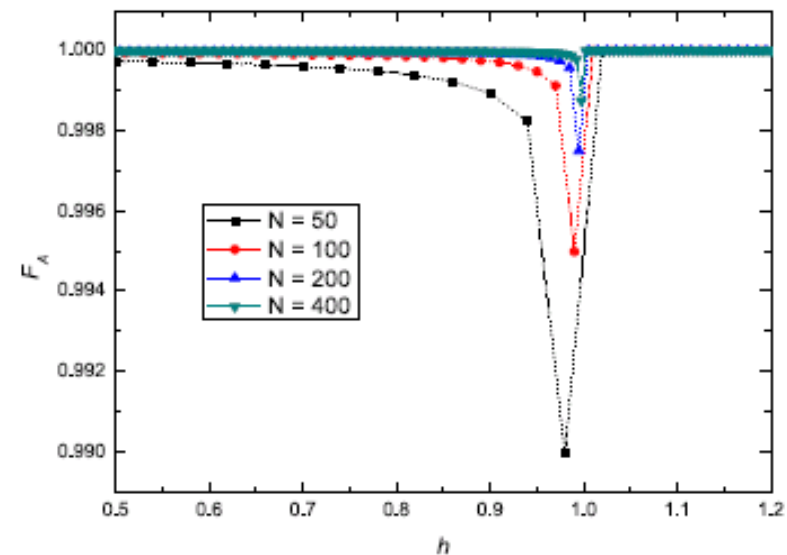
H. N. Xiong, J. Ma, Z. Sun, and X. Wang,
arXiv:0808.1817.



Example: Reduced fidelity

$$\begin{aligned} H_{\text{LMG}} &= -\frac{1}{N} \sum_{i < j} (\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j) - h \sum_i \sigma_z^i \\ &= -\frac{2}{N} (S_x^2 + S_y^2) - 2hS_z + \frac{1}{2} \\ &= -\frac{2}{N} (S^2 - S_z^2 - N/2) - 2hS_z. \end{aligned}$$

$$E(M, h) = \frac{2}{N} \left(M - \frac{hN}{2} \right)^2 - \frac{N}{2} (1 + h^2).$$





Summary

- 1. We establish a general relation between the fidelity and dynamic structure factor of the driving parameter**
- 2. We can learn the universality class of the critical phenomena from the Fidelity susceptibility.**
- 3. Fidelity susceptibility and bond-bond long range correlation can also describe the topological phase transitions.**
- 4. We propose a density-functional fidelity and use reduced fidelity to study the quantum phase transitions**