Polarization in Quantum Many-Body Systems

Topological phases of matter [TOPMAT]:
from the quantum Hall effect to spin liquids
11 juin 2018 @ IPhT CEA Saclay
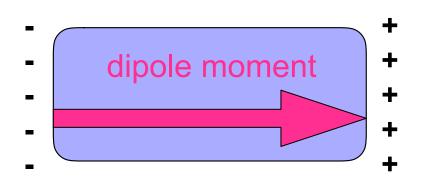
Masaki Oshikawa
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Polarization density

From Wikipedia, the free encyclopedia

In classical electromagnetism, **polarization density** (or **electric polarization**, or simply **polarization**) is the vector field that expresses the density of permanent or induced electric dipole moments in a dielectric material. When

- \- \+
- \- dipole moment \+
- \- \+
- \- \+
- \- \+

polarization density
= bulk property

can be defined with
periodic boundary condition?

Modern Theory of Polarization

by King-Smith and Vanderbilt, Resta et al.
  initial motivation: how to discuss polarization
in band theory with periodic boundary conditions

Theory of polarization of crystalline solids

R. D. King-Smith and David Vanderbilt
Department of Physics and Astronomy, Rutgers University, P. O. Box 849, Piscataway, New Jersey 08855-0849

Macroscopic polarization in crystalline dielectrics: the geometric phase approach

Raffaele Resta

Scuola Internazionale Superiore di Studî Avanzati (SISSA), via Beirut 4, I-34014 Trieste, Italy

The macroscopic electric polarization of a crystal is often defined as the dipole of a unit cell. In

Polarization = Zak Phase

For 1D band insulators

$$\hat{H} = \int_0^L dx \, c_x^\dagger \left[-\frac{1}{2m}\partial_x{}^2 + V_x \right] c_x$$

Bloch theorem ➜ effective Hamiltonian

$$h_k(r)u_k(r) = \epsilon_k u_k(r)$$

$$\mathcal{P}^{\text{Bloch}} \equiv \int_0^{\frac{2\pi}{a}} \frac{dk}{2\pi} \int_0^a dr \, iu_k(r)^*\partial_k u_k(r).$$

Well-defined modulo integer

Haruki Watanabe & M. O.
arXiv:1802.00218

Is the Zak phase unique?

Two ways of Fourier transformation

(I)

$$\hat{c}_x \equiv \frac{1}{\sqrt{L/a}} \sum_{n=1}^{L/a} \hat{c}_{k_n,r} e^{ik_n x}, \quad k_n \equiv \frac{2\pi}{L} n.$$

$$\hat{h}_k \equiv \int_0^a dr \, \hat{c}_{k,r}^\dagger h_{k,r} \hat{c}_{k,r}, \quad h_{k,r} \equiv \frac{-(\partial_r + ik)^2}{2m} + V_r.$$

(II)

$$\hat{c}_x \equiv \frac{1}{\sqrt{L/a}} \sum_{n=1}^{L/a} \hat{\tilde{c}}_{k_n,r} e^{ik_n R}.$$

R: position of the unit cell

$$\hat{\tilde{c}}_{k,r} = e^{ikr} \hat{c}_{k,r}.$$

$$\tilde{h}_{k,r} = e^{ikr} h_{k,r} e^{-ikr}$$

$$\tilde{u}_k(r) = e^{ikr} u_k(r)$$

Two conventions

convention (I)

    natural from Fourier transform in free space

    but $h_{k,r} \equiv \frac{-(\partial_r + ik)^2}{2m} + V_r.$ is NOT periodic in the BZ
and thus u_k is neither.

$$u_{k+\frac{2\pi}{a}}(r) = e^{-2\pi i \frac{r}{a}} u_k(r)$$

    Berry phase??

$$\tilde{u}_k(r) = e^{ikr} u_k(r)$$

convention (II)

    satisfies the periodicity in the BZ
but "twisted boundary condition" in the real space

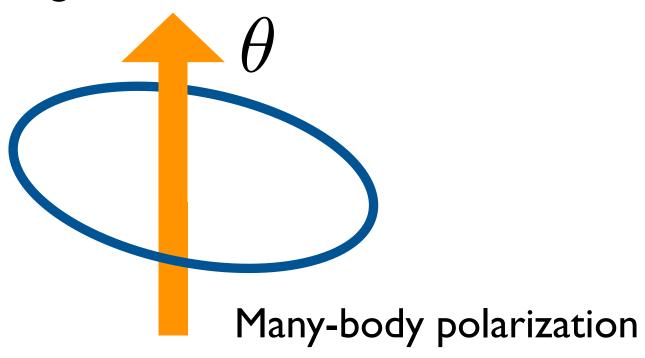$$\tilde{u}_k(r+a) = e^{ika} \tilde{u}_k(r).$$

Two (and More) Polarizations

Are they equivalent?
No.

Then, which one is correct?

Going to Many-Body

change of wavevector ⇔ flux insertion

θ

Many-body polarization

$$\mathcal{P} \equiv \int_0^{2\pi} \frac{d\theta}{2\pi} \, i\langle \Phi_\theta | \partial_\theta | \Phi_\theta \rangle \quad ?$$

Two Different Gauges

Gauge choice (I): uniform gauge

$$A_x = \frac{\theta}{L} \qquad \hat{H}_\theta = \int_0^L dx \; c_x^\dagger \left[-\frac{1}{2m}(\partial_x + i\frac{\theta}{L})^2 + V_x \right] c_x$$

Hamiltonian (and state) not periodic in θ

Gauge choice (II): boundary gauge

$$A_x = \theta \sum_{n \in \mathbb{Z}} \delta(x - nL)$$

equivalent to twisted b.c. in the real space

Two Many-Body Polarizations

Gauge choice (I): uniform gauge

$$\mathcal{P} \equiv \int_0^{2\pi} \frac{d\theta}{2\pi} \, i\langle\Phi_\theta|\partial_\theta|\Phi_\theta\rangle + \mathrm{Im}\ln\langle\Phi_0|e^{2\pi i\hat{P}}|\Phi_{2\pi}\rangle,$$

Gauge choice (II): boundary gauge

$$\tilde{\mathcal{P}} = \int_0^{2\pi} \frac{d\theta}{2\pi} \, i\langle\tilde{\Phi}_\theta|\partial_\theta|\tilde{\Phi}_\theta\rangle. \qquad \mathcal{P} = \tilde{\mathcal{P}} + \bar{\mathcal{P}}_0, \quad \bar{\mathcal{P}}_0 \equiv \int_0^{2\pi} \frac{d\theta}{2\pi} \langle\Phi_\theta|\hat{P}|\Phi_\theta\rangle.$$

$$\hat{P} \equiv \frac{1}{L}\int_0^L dx\, x\hat{n}_x, \quad \hat{n}_x \equiv \hat{c}_x^\dagger \hat{c}_x$$

They respectively correspond to Fourier transform conventions (I), (II) for band insulators

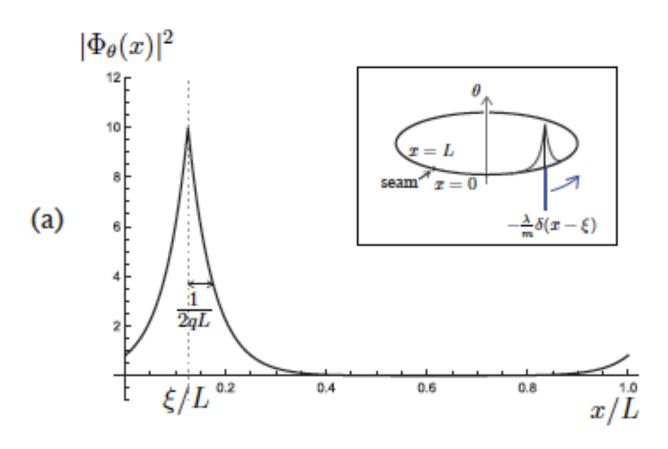# What Do They Represent?

Gauge choice (I): uniform gauge

$$\mathcal{J} = \frac{d\mathcal{P}}{dt} \sim \frac{1}{L} \int_0^L dx \; j(x) \quad \text{averaged current}$$
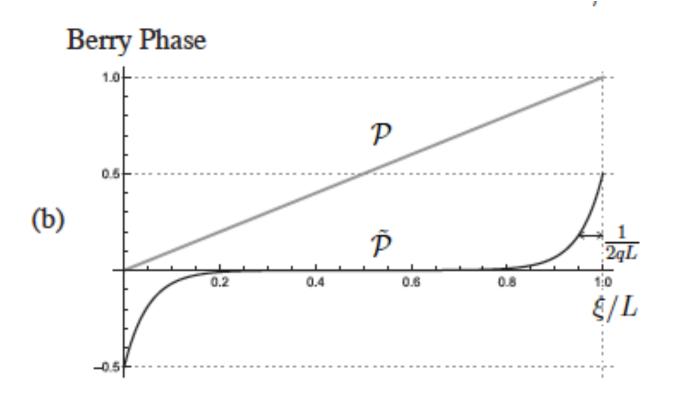
Gauge choice (I): boundary gauge

$$\tilde{\mathcal{J}} = \frac{d\tilde{\mathcal{P}}}{dt} \sim j(0) \qquad \text{local current} \atop \text{at the "seam"}$$
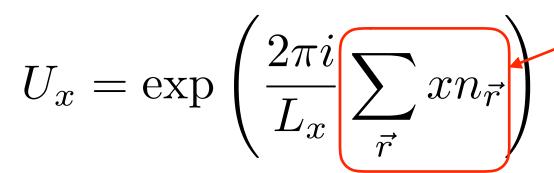
Delta-Function Potential

Delta-Function Potential

$$\int_0^T \mathcal{J} \, dt = \int_0^T \tilde{\mathcal{J}} \, dt = \text{Chern number} = 1$$

Polarization by Resta & Sorella

$\propto$ "center of mass" position of particles

$$U_x = \exp\left(\frac{2\pi i}{L_x}\boxed{\sum_{\vec{r}} x n_{\vec{r}}}\right)$$

L_x : length of system in x-direction

$$z_x = \langle U_x \rangle = |z_x|e^{2\pi i \mathcal{P}_x}$$

total current
$$I_x = e\frac{d\mathcal{P}_x}{dt}$$

$\mathcal{P}_x \quad \propto$ polarization, defined modulo integer

U_x is **exactly identical** to the **LSM-twist** or the **large gauge transformation** operator! (pointed out by Nakamura and Voit, 2002)

Resta-Sorella vs. Berry Phase

$$\mathcal{P}_{\mathbf{R}} \equiv \frac{1}{2\pi}\mathrm{Im}\ln\langle\Phi|e^{2\pi i\hat{P}}|\Phi\rangle,$$

$$\langle\Phi_{2\pi}|\Phi_0\rangle \simeq \langle\Phi_{2\pi}|\Phi_\pi\rangle\langle\Phi_\pi|\Phi_0\rangle$$
$$\simeq \langle\Phi_{2\pi}|\Phi_{\frac{3}{2}\pi}\rangle\langle\Phi_{\frac{3}{2}\pi}|\Phi_\pi\rangle\langle\Phi_\pi|\Phi_{\frac{1}{2}\pi}\rangle\langle\Phi_{\frac{1}{2}\pi}|\Phi_0\rangle$$
$$\simeq \prod_{n=0}^{N-1}\langle\Phi_{\theta_{n+1}}|\Phi_{\theta_n}\rangle, \quad N = 2^M. \qquad (\,$$

$$\mathcal{P}_{\mathbf{R}} = \frac{1}{2\pi}\mathrm{Im}\ln\langle\Phi_{2\pi}|\Phi_0\rangle = \mathcal{P}$$

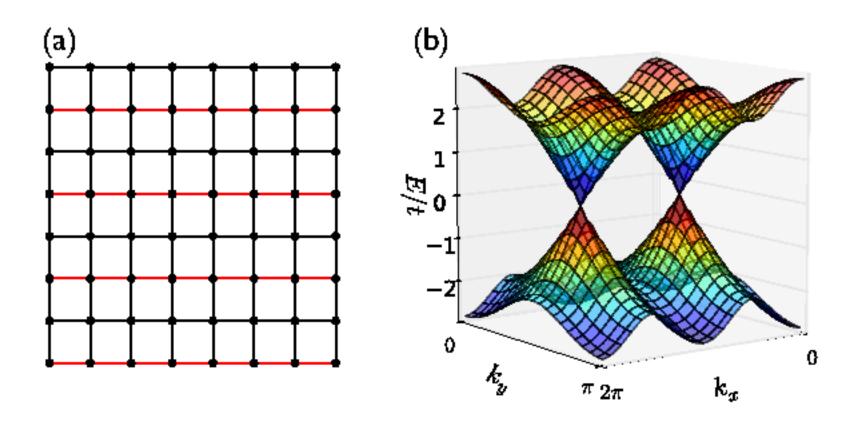rigorously in *d*=1, perhaps in *d*=2

Applications to *d*=2

- Torus version of Laughlin's gauge argument: quantization of Hall conductance without edge state (adiabatic process for gapped QH state)

- Periodic boundary condition enables
  combination of Laughlin + LSM:

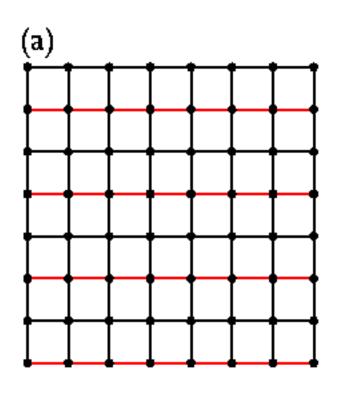$$\tilde{\sigma}_{xy}\phi - \bar{\rho} \in \mathbb{Z}$$

Generalization of the free electrons result by Dana-Avron-Zak 1985 (TKNN formula, Diophantine equation)

Square lattice with π-flux

(a)

(b)

Free fermion dispersion:
        "gapless Dirac points" at half-filling
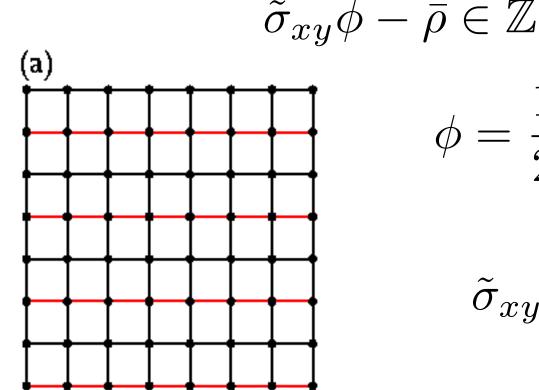
Square lattice with π-flux

(a)

2 sites / unit cell

half-filled:
   1/2 particle / site
   1 particle / unit cell

**NO constraint from
LSM theorem!**

Square lattice with π-flux

$$\tilde{\sigma}_{xy}\phi - \bar{\rho} \in \mathbb{Z}$$

(a)

$$\phi = \frac{1}{2} \qquad \bar{\rho} = \frac{1}{2}$$

$$\tilde{\sigma}_{xy} = \text{odd integer}$$

$$\neq 0$$

Time Reversal invariance must be (spontaneously) broken! ⇒ ground-state degeneracy

Why are insulators insulating and metals conducting?
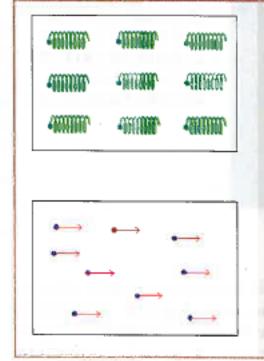
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◄ **Fig. 1:** Schematic view of insulators and metals in classical physics. Top sketch: Lorentz model for insulators, where each electron is tied (by an harmonic force) to a particular center. Bottom sketch: Drude model for metals, where electrons roam freely over macroscopic distances, hindered only by atomic scattering potentials.

Resta-Sorella criterion:

$$\langle U_x \rangle \to z \neq 0$$

insulator (polarization is well-defined)

$$\langle U_x \rangle \to 0 \quad \text{[in the thermodynamic limit]}$$

conductor (polarization is ill-defined)

Scaling of the polarization amplitude in quantum many-body systems in one dimension

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thanks to Gil-Young Cho (POSTECH)

How "good" is the conductor?

conductor (polarization is ill-defined)

$$\langle U_x \rangle \to 0$$

But how "fast"? Perhaps scaling of the many-body polarization…

$$\langle U_x \rangle \sim \left(\frac{1}{L} \right)^{\beta}$$

1D XXZ chain (and its variants)

$$\mathcal{H} = J_1 \sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right)$$

$$+ J_2 \sum_j \left(S_j^x S_{j+2}^x + S_j^y S_{j+2}^y + \Delta S_j^z S_{j+2}^z \right)$$

can be regarded as an interacting spinless boson (or fermion) system

gapless Tomonaga-Luttinger Liquid for $\quad -1 < \Delta \leq 1$

Caveat

$$T_x = e^{iP_x}$$
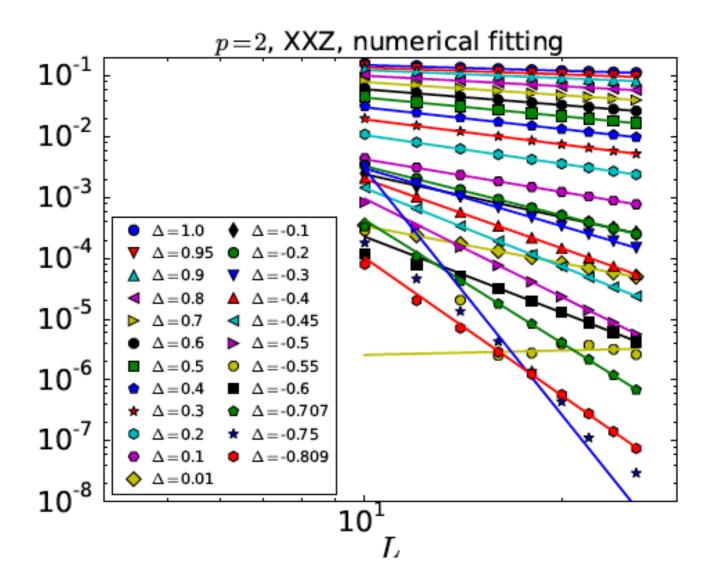
Lattice translation / crystal momentum

$$U_x T_x = T_x U_x e^{2\pi i \nu} \qquad \nu = S - m = \frac{1}{2}$$

$$U_x |\Psi_0\rangle$$

has the crystal momentum different by π
from the original ground state

$$\langle \Psi_0 | U_x | \Psi_0 \rangle = 0$$

So, let us use $\langle \Psi_0 | (U_x)^q | \Psi_0 \rangle$ instead

Aligia-Ortiz 1999

$p=2$, XXZ, numerical fitting

Legend:
- $\Delta=1.0$
- $\Delta=0.95$
- $\Delta=0.9$
- $\Delta=0.8$
- $\Delta=0.7$
- $\Delta=0.6$
- $\Delta=0.5$
- $\Delta=0.4$
- $\Delta=0.3$
- $\Delta=0.2$
- $\Delta=0.1$
- $\Delta=0.01$
- $\Delta=-0.1$
- $\Delta=-0.2$
- $\Delta=-0.3$
- $\Delta=-0.4$
- $\Delta=-0.45$
- $\Delta=-0.5$
- $\Delta=-0.55$
- $\Delta=-0.6$
- $\Delta=-0.707$
- $\Delta=-0.75$
- $\Delta=-0.809$

L

$p=2$, XXZ, exponent by numerical fit

fit result
$4K-2$

$K = \pi/(2\cos^{-1}(-\Delta))$
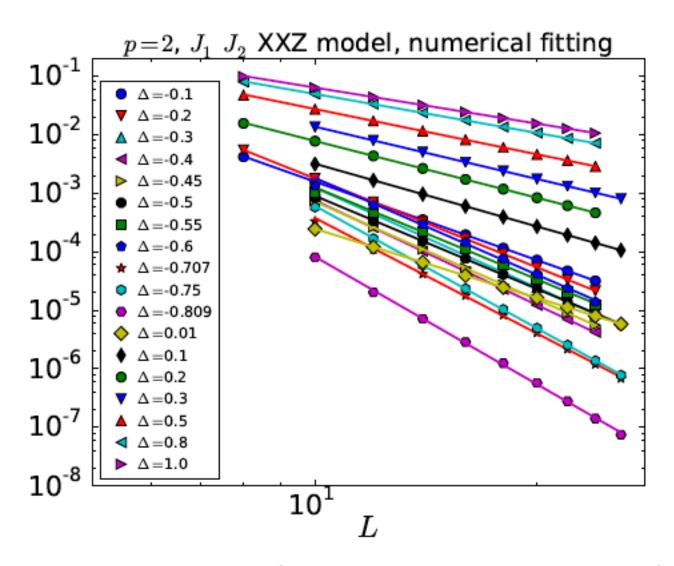
$\beta = 4K - 2$?

XY chain = free fermion point

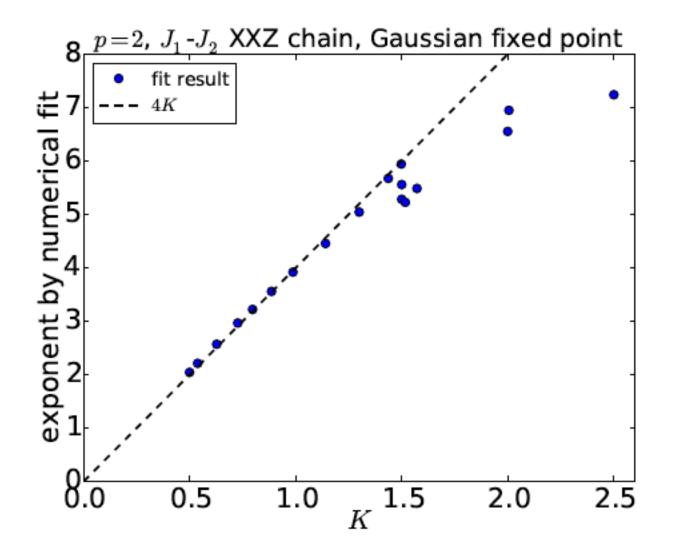$$\langle \Psi_0 | \, (U_x)^q \, | \Psi_0 \rangle = 0 \qquad \text{for free fermions}$$

What makes it non-zero for interacting systems?

Umklapp scattering?

We can make the leading Umklapp vanishing by tuning J_2!

$p=2$, J_1 J_2 XXZ model, numerical fitting

Indeed, it vanishes faster in the absence of the leading Umklapp….

$p=2$, J_1-J_2 XXZ chain, Gaussian fixed point

$\beta = 4K$?
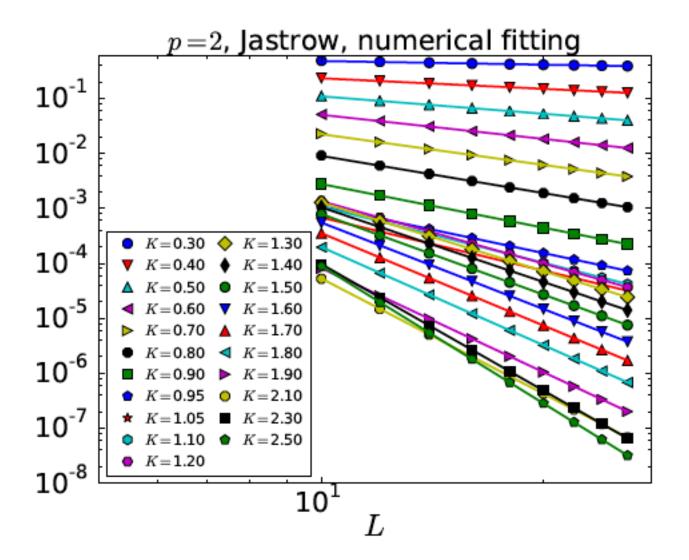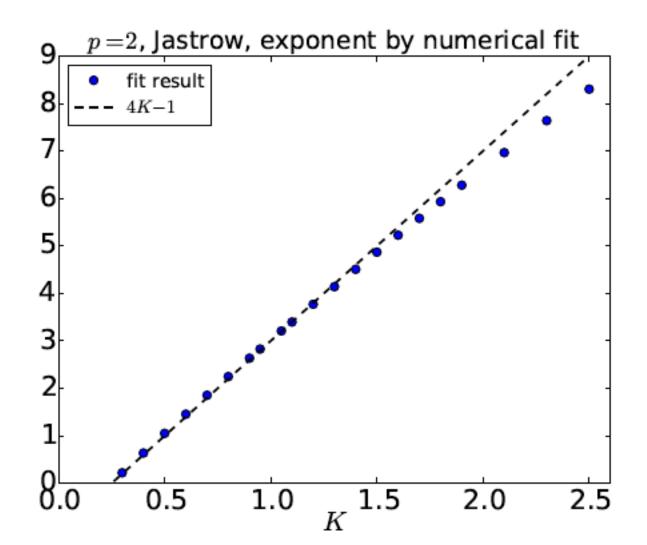
(cf. $\beta = 4K - 2$ in XXZ)

Haldane-Shastry model

$1/r^2$ interaction: exact Jastrow-type groundstate

$$\tilde{\Psi}_G(x_1, \ldots, x_M) = \prod_i z_i^{-\frac{L(L-1)}{4K}} \prod_{i<j} (z_i - z_j)^{\frac{1}{K}}$$

"ideal" realization of CFT: all the Umklapp vanish?
⇒ expectation value should vanish very quickly

if it is not exactly zero???

$p=2$, Jastrow, numerical fitting

Legend:
- $K=0.30$
- $K=0.40$
- $K=0.50$
- $K=0.60$
- $K=0.70$
- $K=0.80$
- $K=0.90$
- $K=0.95$
- $K=1.05$
- $K=1.10$
- $K=1.20$
- $K=1.30$
- $K=1.40$
- $K=1.50$
- $K=1.60$
- $K=1.70$
- $K=1.80$
- $K=1.90$
- $K=2.10$
- $K=2.30$
- $K=2.50$

$p=2$, Jastrow, exponent by numerical fit

- fit result
- - - $4K-1$

$\beta = 4K - 1$???

(cf. $\beta = 4K - 2$ in XXZ

$\beta = 4K$ in J_1-J_2)

Exact Result for H-S model

at SU(2) point:

$$\langle \Psi_0 | (U_x)^2 |\Psi_0\rangle = \frac{1}{L-1}$$

$$\langle \Psi_0 | (U_x)^{2n} |\Psi_0\rangle = \frac{(2n-1)!!(L-2n-1)!!}{(L-1)!!}$$

(by combinatorics)

Finite-size scaling of MBP amplitude

▸ Confirmed power-law scaling in *XXZ* chain
  (and its generalizations)
▸ However, the exponent seems "non-universal"
  (different for XXZ, J_1-J_2, Haldane-Shastry)
▸ No field theory understanding??
▸ Non-universal nature is related to the
  quantum quench? (sudden flux insertion)
▸ Modified quantity might show
  more universal behavior??