# Division Report, 2017

H.Q. Lin (林海青)

Thanks to: Colleagues, Postdoctoral, Students, Associate Members & Visitors, Miss Wei Liu & Administration Staff, etc.

**Research Area: Condensed Matter, Computational Physics, …**
**Modeling and Computing**
**1st principles calculations, Green Function, Exact Diagonalization, Monte Carlo Simulation, Tensor Network, etc.**
**FDTD, etc.**



2017-10-16, Sao Paulo

# Outline

- Division Profile
- Faculty Members and Research Projects
- …

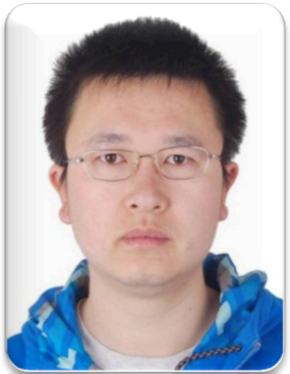
# Division Profile (2016.01-Present)

| Content | Progress |
|---|---|
| Faculty Members | Hai-Qing Lin, Wen Yang, Dong-Bo Zhang, Stefano Chesi, Ling Wang (2015-08), Rubem Mondaini (2016-01) |
| Publications | 93 Total Publications; 18 Publications with IF > 5.0; 23 with CSRC as First/Corresponding Author Address |
| Research Grants | Ongoing Projects: 15; Completed Projects: 7 |
| Supervision | Postdocs (Current/Left/Coming): 20/6/1<br>Students (Current/Graduated/Coming): 6/2/5 |
| Academic Exchanges | Hosting Visitors : >130<br>Workshops/Conferences Attended: 52 |
| Division Activities | Joint Group Meetings (Weekly)<br>Two Workshops |

Webpage: http://www.csrc.ac.cn/en/about_csrc/organization/simulation_of_physical_system/

# Faculty Members

林海青 (Hai-Qing Lin)
Chair Professor
Division Head



杨文 (Wen Yang)
Assistant Professor

张东波 (Dong-Bo Zhang)
Assistant Professor

Stefano Chesi
Assistant Professor

汪玲 (Ling Wang)
Assistant Professor

Rubem Mondaini
Research Assistant Professor

# Hai-Qing Lin's Group

## Hai-Qing Lin's Group:

**PI**: Hai-Qing Lin, 2012-09, 1000 Talents Plan; PhD, UC San Diego

**Research Interests**: Condensed Matter Physics and Computational Physics including plasmonics, high pressure studies, entanglement and quantum phase transition, magnetism and superconductivity, electron spins in semiconductor quantum dots as well as numerical technique development.

**Postdocs**: Wei Wu;

**Co-Supervision**: *Da-Wei Luo, Hui Shao, Tilen Cadez*

**Students**: **Ya-Ming Xie, Xiao-Hui Wang**, Sheng-Wen Li, Jian Li (2016-09)

# Research Interests

- **Superconductivity & Magnetism**
  - Effects of Electron-Electron Correlations
  - Effects of Electron-Phonon Interactions
  - Orbital Physics
- **Quantum Phase Transitions**
- **Quantum Information**
- **Optical Properties of Nanostructure**
- **Numerical Techniques: QMC, etc.**
- **…**

# Wilson Ratio

**Wilson Ratio** $$\lim_{T\to 0} \frac{C(T)}{T\chi(T)} = \frac{4\pi^2 k^2}{3R},$$ ***R* = constant**

**K. G. Wilson, RMP 47, 773 (1975)**

TABLE XV. Results of the Kondo calculation.

| $\Lambda$ | 2.0 | 2.25 | 2.5 | 3 |
|---|---|---|---|---|
| $R$ | 1.998 | 1.9994 | 2.00006 | 2.0001 |
| $\chi_z$ | 0.10345 | 0.10315 | 0.1029 | 0.1026 |
| $N_i$ | 43 | 35 | 31 | 31 |
| $z_i$ | 0.0408546 | 0.0409743 | 0.0417065 | 0.0303433 |
| $N_f$ | 142 | 130 | 114 | 120 |
| $E_{1f} - E_1(\infty)$ | $-2.2027 \times 10^{-5}$ | $-2.5359 \times 10^{-6}$ | $-1.3746 \times 10^{-5}$ | $-2.5902 \times 10^{-4}$ |

**Collective Excitation:**

**conduction electron + impurity → spin singlet**

# Wilson's Renormalization Group

**1982 Nobel Prize**

- Find the deep understanding of RG method.
- Give the explicit formulae of RG theory.
- Solve the Kondo problem.

# Wilson Ratio

**Fermi liquid** 3D $c_V = \frac{1}{3}\frac{m^* k_F k_B^2 T}{\hbar^3}$, $\chi = \frac{m^* k_F}{\pi^2 \hbar}\frac{\mu_F^2 g^2}{1+F_0^a}$, $R_W = \frac{1}{1+F_0^a}$

**Luttinger liquid** 1D $c_V = \frac{\pi k_B^2 T}{3\hbar}\left(\frac{1}{v_s}+\frac{1}{v_c}\right)$, $\chi = \frac{1}{\hbar \pi v_s}$, $R_W = \frac{2v_c}{v_c + v_s}$

| Model | Wilson Ratio R |
|---|---|
| 3D Kondo problem, Kondo regime | $R_w$~2 T<<$T_K$ |
| 3D noninteracting or weakly interacting electrons in metal | $R_w$~1 |
| 1D strong repulsion limit | $R_w$~2 |
| 1D free fermions limit | $R_w$~1 |

- $R_w > 1$ in strongly correlated systems where spin fluctuations are enhanced while charge fluctuations are suppressed.
- $R_w = 2$ for 1D spin-1/2 Heisenberg chain.

# Wilson Ratios

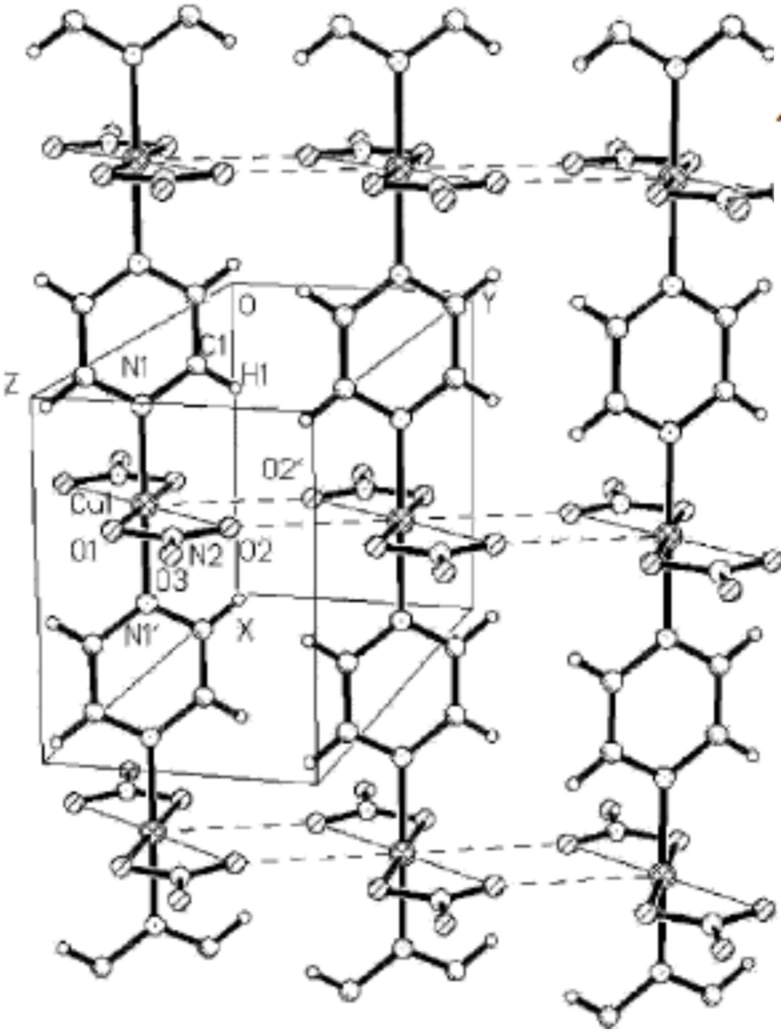
The Wilson ratios, defined as **the ratios of the magnetic susceptibility/compressibility to specific heat divided by temperature** are dimensionless constants at the renormalization fixed point of these systems. The values of the ratio indicate interaction effects and quantities spin/particle number fluctuations, relatively easy to measure.

**Gibbs Energy:** $G = E - N\mu - MH - TS$

**Spin fluctuation:** $\langle \delta M^2 \rangle = \Delta^D k_B T \chi \quad R_W^s = \frac{4k_B^2\pi^2}{3(\mu_B g)^2} \frac{\chi}{c_v/T}$

**Particle number fluctuation:** $\langle \delta N^2 \rangle = \Delta^D k_B T \kappa \quad R_W^c = \frac{\pi^2 k_B^2}{3} \frac{\kappa}{c_v/T}$

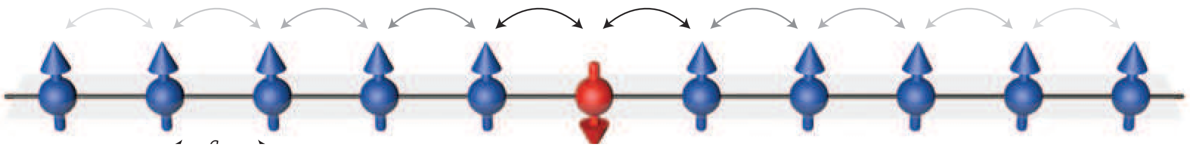
# CuPzN (Cooper pyrazine dinitrate)




$$\mathcal{H} = J \sum_{j=1}^{N} \vec{S}_j \cdot \vec{S}_{j+1} - g\mu_B H \sum_{j=1}^{N} \vec{S}_j^{\,z}$$

1D spin-1/2 chain with
intrachain $J \approx$ 10.8K,
interchain $J' \approx$ 0.046K
PRB 59, 1008 (1999);
PRL 114, 037202 (2015).

We study this system numerically & analytically.



Bethe ansatz equations :
$$\left(\frac{\lambda_j - \frac{i}{2}}{\lambda_j + \frac{i}{2}}\right)^N = -\prod_{l=1}^{M} \frac{\lambda_j - \lambda_l - i}{\lambda_j - \lambda_l + i}$$

energy :
$$E(\lambda_1, ., \lambda_M) = -\sum_{j=1}^{M} \frac{J}{\lambda_j^2 + \frac{1}{4}} + HM + \frac{1}{2} N (J - H)$$

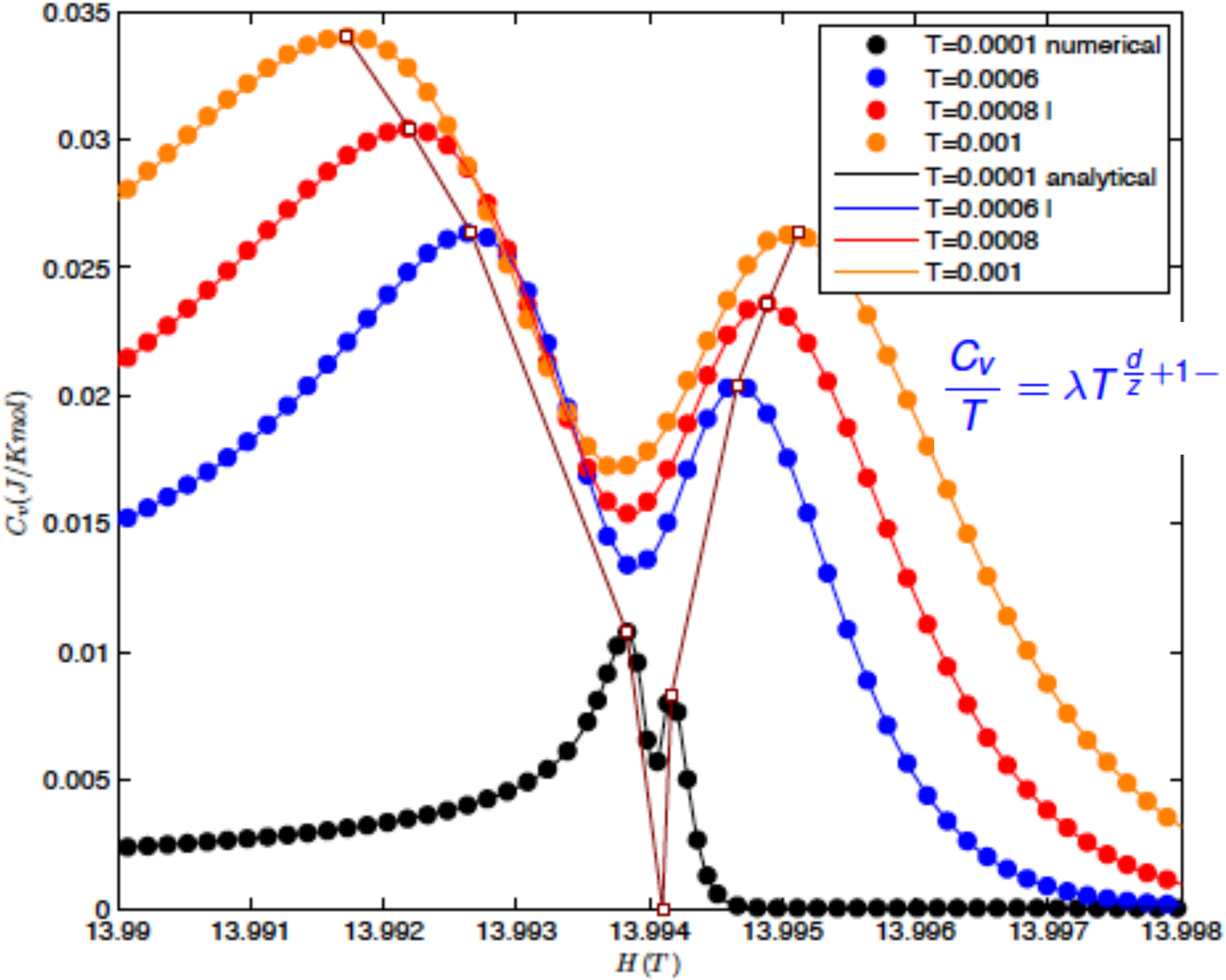
thermodynamics Bethe ansata :
$$\ln(1 + \eta_n) = \frac{\varepsilon_n^0}{T} + \sum_m A_{m,n} * \ln\left(1 + \eta_m^{-1}\right)$$

$$\varepsilon_n^0 = -2\pi a_n + nH, \quad n = 1, \ldots, \infty$$

free energy :
$$f = -T \sum_n \int a_n(\lambda) \ln\left(1 + \eta_m^{-1}(\lambda)\right) d\lambda$$

Bethe, 1931, Z. Phys. 71, 205
Yang and Yang, PR 150, 321 (1966); PR 150, 327 (1966); PR 151, 258 (1966)
Takahashi, Thermodynamics of One-Dimensional Solvable Models (Cambridge: Cambridge University Press) 1999

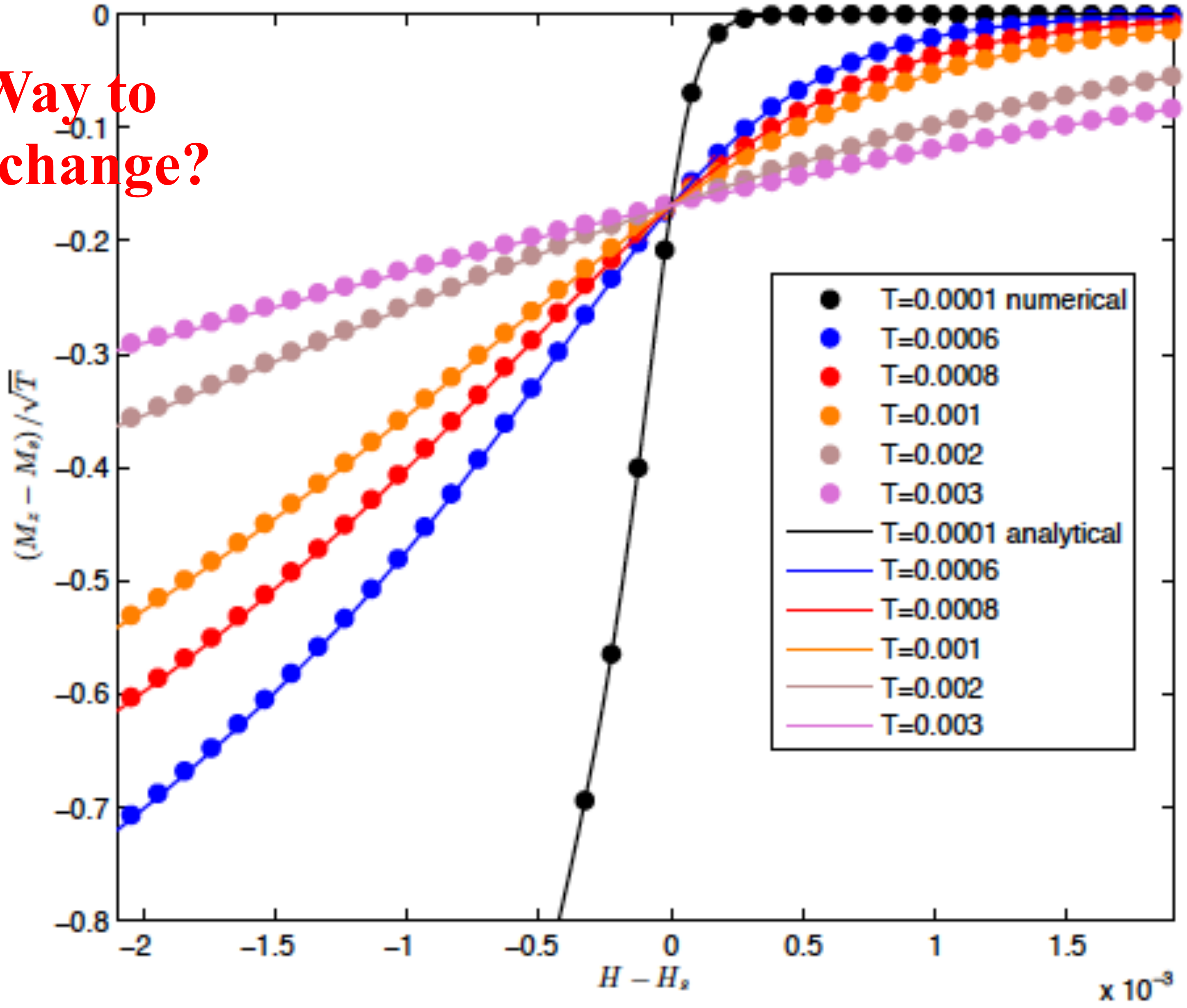
# $CuP_zN$: the specific heat vs $H$

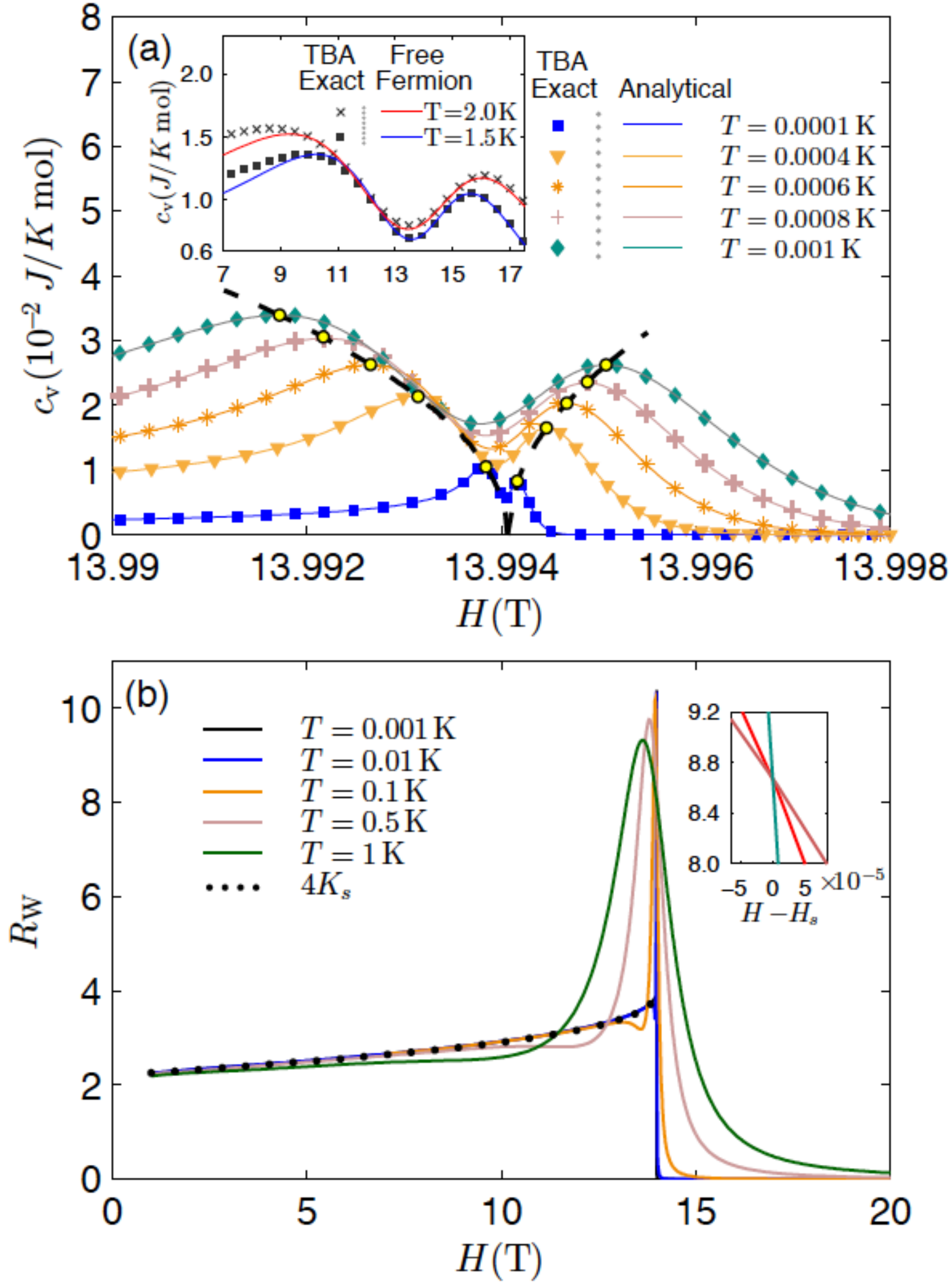



$$\frac{C_V}{T} = \lambda T^{\frac{d}{z}+1-\frac{1}{\upsilon z}} \mathcal{C}\left(\frac{H-H_s}{T^{\frac{1}{\upsilon z}}}\right)$$

# $CuP_zN$: critical properties

**Easy Way to phase change?**



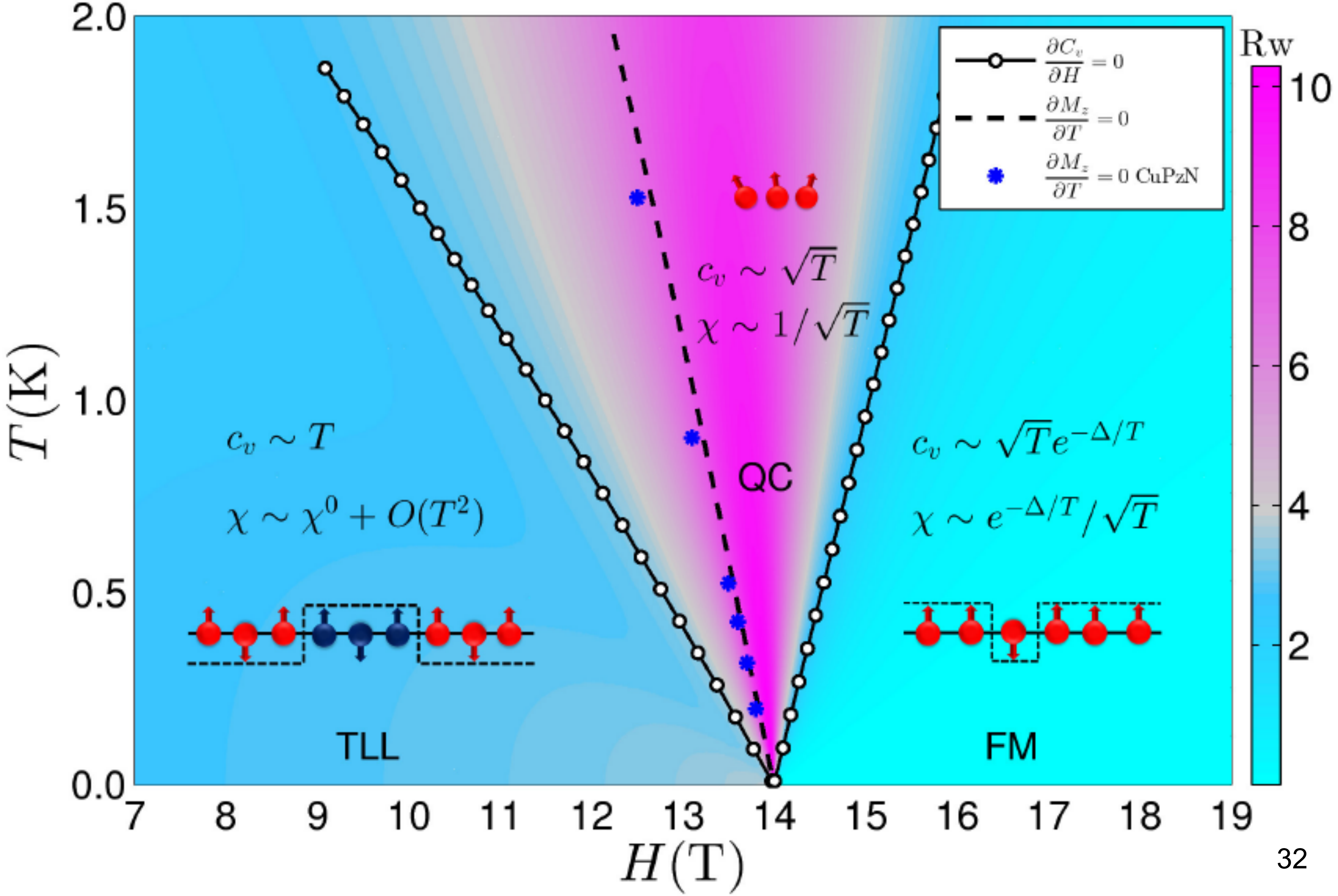



(a) Numerical and analytical specific heat vs magnetic field. The double-peaks (circles) fanning out from the Hs = 13.9941(T) mark the crossover temperatures separating the three regions: the TLL, the QC and the FM.

(b) The numerical plot of the Wilson ratio at different temperatures, which collapse to the Luttinger parameter curve of 4Ks, indicating the TLL nature.

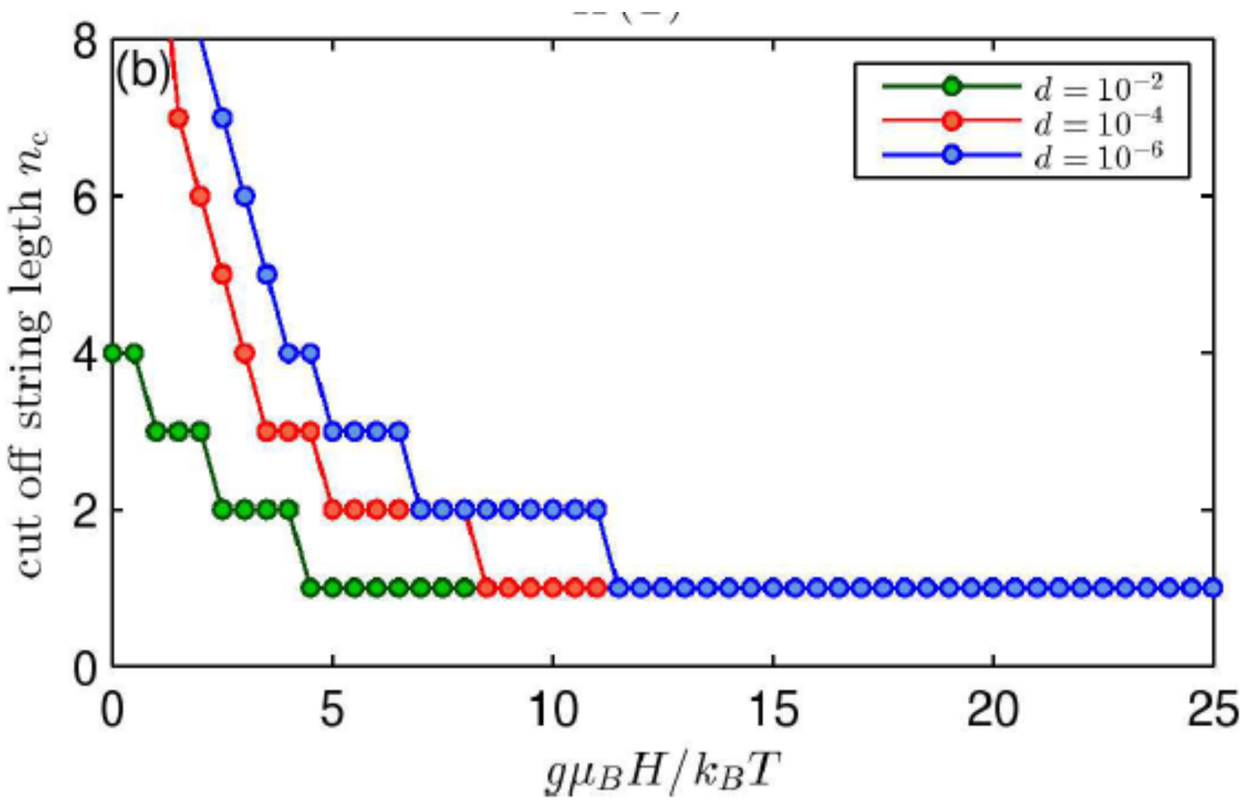
The inset shows an intersection of the Wilson ratio curves at low temperatures.

# Wilson ratio in the 1D Heisenberg Chain



# Quantum Criticality of Spinors

- Elementary excitation S=1 => 2 S=1/2 spinors.
- String length *n*: $\lambda_{j,\ell}^{n} = \lambda_{j}^{n} + \mathrm{i}(n+1-2\ell)$



# Quantity to Measure

- Physics is an experimental science, what to measure is essential in reveling the underline mechanism;
- Considering complexity of the system and fluctuations and errors in the measurements, it is preferable to measure thermodynamic quantities who depend on external variables weakly;
- Wilson ratio is such a quantity.

# 2-Component Fermi Gas

## Gaudin-Yang model:

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + g_{1D}\sum_{i=1}^{N_\uparrow}\sum_{j=1}^{N_\downarrow}\delta(x_i - x_j) + E_z$$

$$E_z = -(1/2)g\mu_B H(N_\uparrow - N_\downarrow)$$

$$g_{1D} = -(2\hbar^2/ma_{1D})$$ $H = \mu_{\uparrow} - \mu_{\downarrow}$ external

$$c = mg_{1D}/\hbar^2$$ $\gamma = c/n$ interaction

$c$ measures interaction strength.

Analytically, we could perform *c- or 1/c*-expansion



**Guan, Yin, Foerster, Batchelor, Lee, Lin, PRL 111, 130401 (2013).**

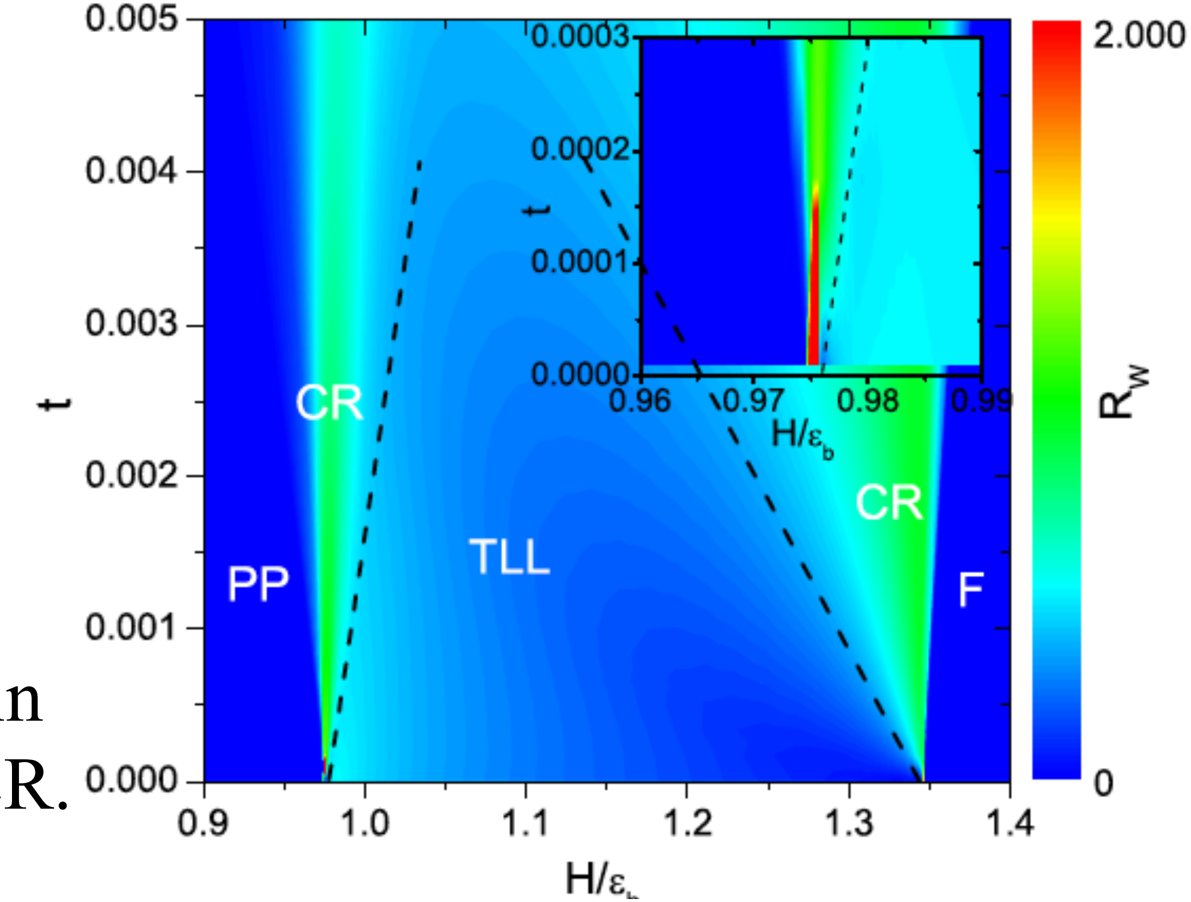
# 2-Component Fermi Gas

$|\gamma| = 10$

$t$: temperature $T/\varepsilon_b$

$R_W = 0$ for PP (pairs) and F (unpaired)

$R_W$ shows $T$-dependent scaling in the critical regimes CR.




Inset: near critical points, anomalous enhancement

$$R_W = \frac{4}{(v_N^b + 4v_N^u)(\frac{1}{v_s^b} + \frac{1}{v_s^u})}$$



**Guan, Yin, Foerster, Batchelor, Lee, Lin, PRL 111, 130401 (2013).**

# 2-Compo

## Wilson ratio $R_w^c$ & the phase diagram

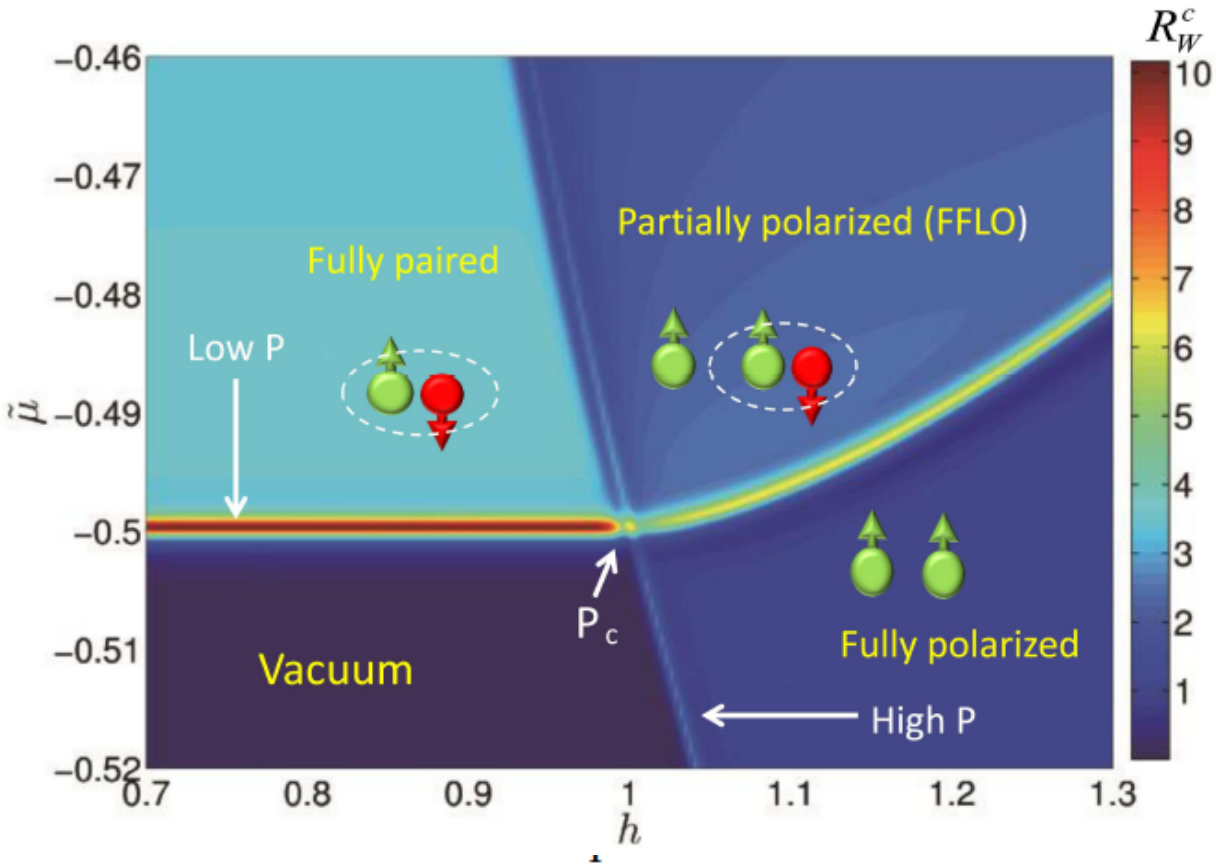
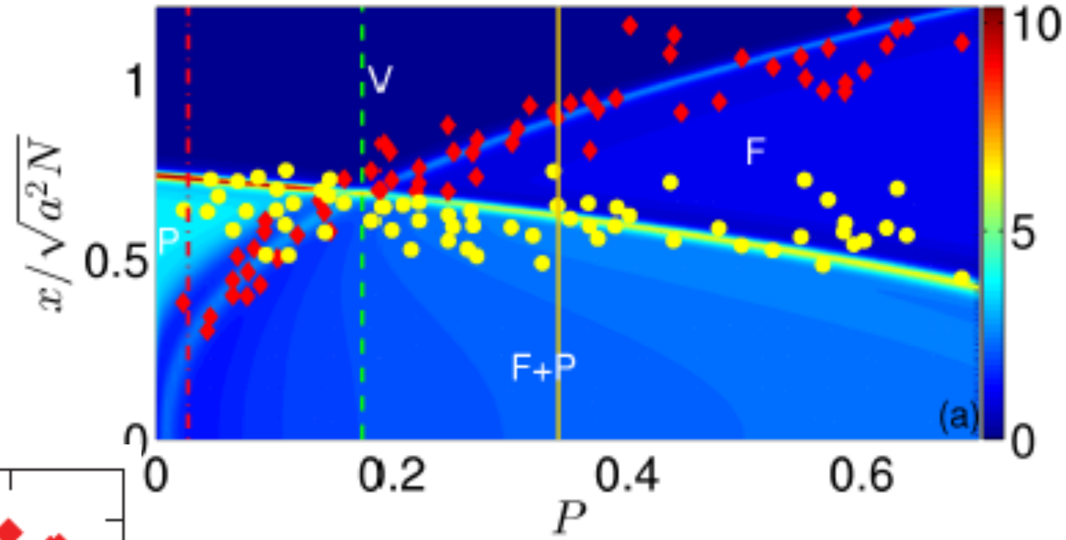


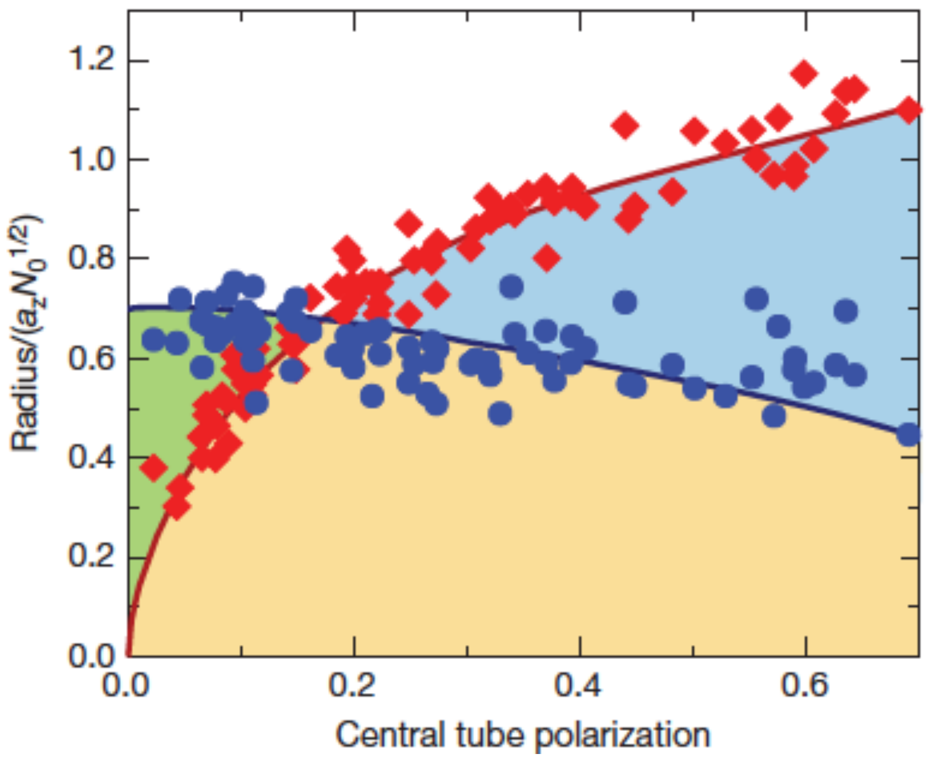

FIG. 1: Contour plot of the
temperature $T = 0.001\varepsilon_2/k_B$
bound pair. Here $\tilde{\mu}$ and $h$ are
and magnetic field. The Wilson ratio gives different constant values which characterize three Luttinger liquid phases of fully-paired state, partially-polarized FFLO like state and the fully-polarized normal Fermi gas. The Ratio near four different phase boundaries exhibits universal scaling behaviour, see the text in this Supplementary Material. In this figure, $P_c$ stands for the critical polarization. The low (high) $P$ denote the low (high) polarization. The polarization is defined by $P = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow)$. The Wilson ratio remarkably displays two distinct plateaus of the integers 1 and 4 in strong coupling limit.

# 2-Component Luttinger Liquid

**Wilson ratio $R_w^c$ & the phase diagram**




**Yu, Chen, Roemer, Lin, Guan, arXiv:1508.00763**




**Two-component ultracold $^6$Li;**
**Liao et al, Nature 467, 567 (2010)**

# Why Wilson Ratio?

- Provides the opportunity to probe and understand the universal nature of complicated many-body systems by measuring the Wilson ratio, **a single quantity**.
- The Wilson ratio has recently been measured in experiments on a gapped spin-1/2 Heisenberg ladder, K. Ninios, T. Hong, T. Manabe, C. Hotta, S.N. Herringer, M.M. Turnbull, C.P. Landee, Y. Takano, and H.B. Chan, PRL 108, 097201 (2012); Possible for other 1D gas, e.g., $^{6}Li$ atoms.
- Fermi liquid, Luttinger liquid, Spin liquid, Bosons, mixture of cold atoms with higher spin symmetry, etc. could all be discussed on the same foot.