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Density Functional Theory and Quantum Phase Transitions

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A simple discussion of key conceptual ideas

1. Quantum Phase Transition
2. Density Functional Theory
3. Entanglement by DFT to detect QPT

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Quantum Phase Transitions

- What is QPT?
  - Hamiltonian $H = H_0 + H_1(\lambda)$
  - QTP across $\lambda = \lambda_c$, a non-analytic point of GS $E(\lambda)$.
- Reasons for interest in QPT
  - Limit of thermal or classical phase transition
    - (QPT may not always be such a limit.)
  - Suits simulation with optical lattices of atoms
  - QPT in d dimen <==> Scaling in CPT in d+1
    - Scaling solutions in d+1 Ising model ==> QPT in d
    - Imagine quantum computation of d quantum Ising model ==> CPT scaling in d+1
  - Adiabatic quantum computation (a hindrance?)

Sachdev, Quantum Phase Transitions (CUP, 1999)

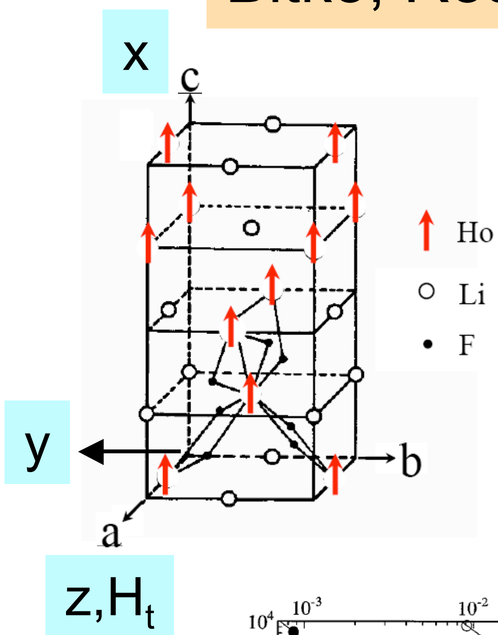
Theoretical example: transverse field Ising model

- $H_0 = -J \sum_i \sigma_i^x \sigma_{i+1}^x$
  - Ising model with ferromagnetic interaction along ±*x*
- $H_1 = -\lambda J \sum_i \sigma_i^z$
  - in the transverse field +*z* direction.
- Quantum critical point at $\lambda_c = 1$ (exact solution).
- $\lambda < 1$, two degenerate magnetically ordered states
- $\lambda > 1$, quantum paramagnet with short range correlation

Sachdev, Quantum Phase Transitions (CUP, 1999)

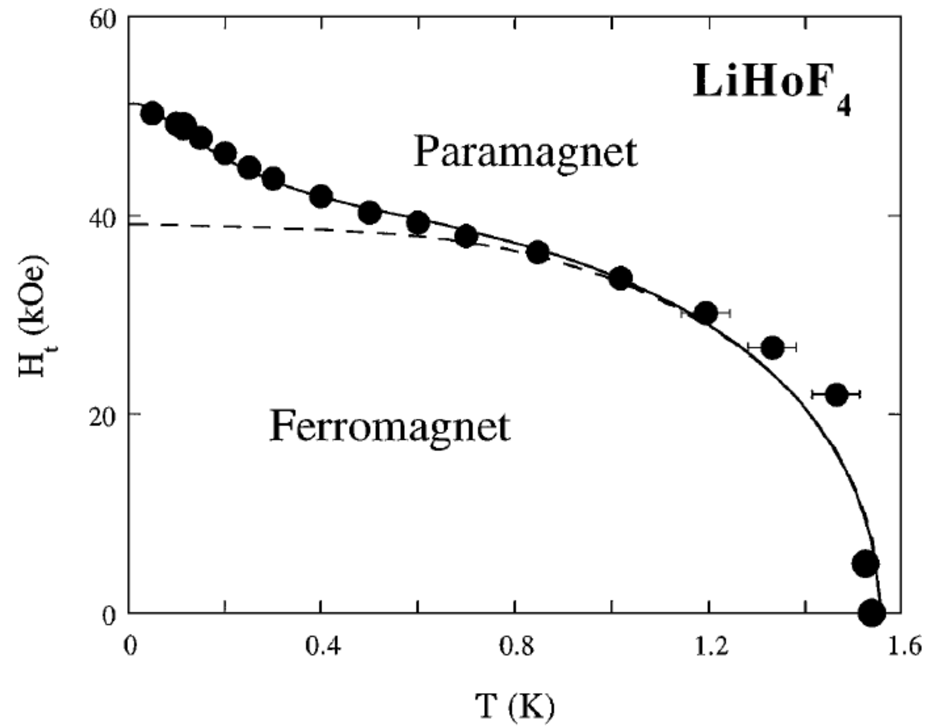
Experimental Example of Transverse Ising Model + Dipolar

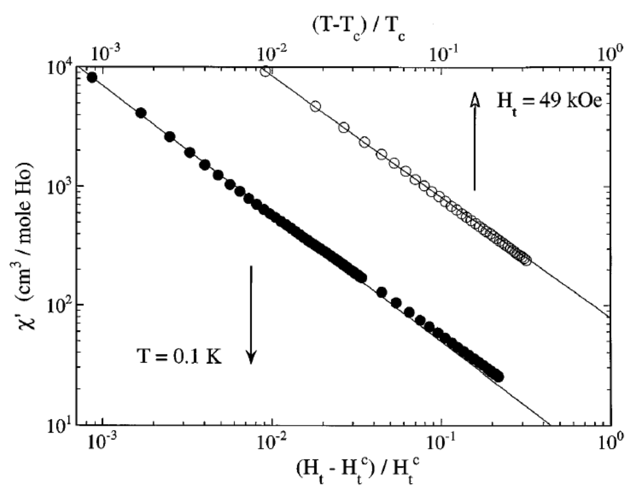
Bitko, Rosenbaum & Aeppli, PRL **77**, 940 (1996)



$LiHoF_4$

Interface fluctuation quantum dot





Behavior mean-field like

Critical behavior from susceptibility meas

Density Functional Theory - I

Legendre transformation $E = U - HM;\ dU = TdS + HdM;\ dE = TdS - MdH$

Density Functional Theory Hohenberg, Kohn, Sham

System of interacting particles $\mathbf{H} = \mathbf{H}_0 + \int dr\, \mathbf{v}(r)\, \hat{\mathbf{n}}(r)$

Non-degenerate ground state: energy $E = \int dr\, v(r)\, n(r) + F[n]$

$n(r)$ = ground state density distribution

$F[n]$ determined entirely by $n(r)$

Any property as a functional of v(r) may be transformed to a functional of n(r).

If the ground state is degenerate,

find the responsible symmetry and break it before applying DFT.

Generalization of Density Functional Theory

Hamiltonian $H_0 + H_1 = H_0 + \sum_i \lambda_i \hat{A}_i$

Observable ~ $\hat{n}(r)$

Interacting particles or spins

External field parameter ~ v(r)

i = lattice site index

Local observables $[\hat{A}_i , \hat{A}_k] = 0$ but $[\hat{A}_i , \hat{B}_i] \neq 0$ is OK

$\hat{A}_i \hat{A}_{i+k}$ is "local" for a fixed k

Ground state expectation values $a_i = \langle \psi | \hat{A}_i | \psi \rangle$

A property is a function of the whole set of parameters λ_i.
It may be transformed to a function of the set $\{a_i\}$.

Instead of generating the QP diagram by varying the fields $\{l_i\}$, one may vary the "magnetizations" $\{a_i\}$.

$$\frac{\partial E}{\partial \lambda_l} = \langle \psi | \frac{\partial H}{\partial \lambda_l} | \psi \rangle = \langle \psi | \hat{A}_l | \psi \rangle = a_l$$

Density Functional Theory - II

Variational principle wrt n(r)

$E = \int dr\, v(r)\, n(r) + F[n]$

$v(r) + \delta F[n]/\delta n = \mu$ ← Fermi energy

$v(r) + \delta T_s[n]/\delta n + \delta E_{xc}[n]/\delta n = \mu$

Single particle KE

Exchange & correlation energy for femions

Single particle Schrödinger eq. with effective potential:

$v(r) + \delta E_{xc}[n]/\delta n$ will have the same variational equation.

Approximations such as local density approximation possible

Entanglement and QPT

In the vicinity of the quantum critical point

Correlation length scales with the coupling parameter, $\xi \propto |\lambda - \lambda_c|^{-\nu}$

Entanglement is a quantum correlation. It may scale near QCP.

DFT to compute entanglement: valid local terms

Transverse field Ising model

$$H = -J\left(\sum_i \sigma_i^x \sigma_{i+1}^x + \lambda \sum_i \sigma_i^z \right)$$

XXZ

$$H(\Delta) = \sum_l \left[\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y + \Delta \sigma_l^z \sigma_{l+1}^z\right]$$

field parameter

NOT for XYX(z)

$$H = \sum_{\langle ij \rangle} \left[S_i^x S_j^x + \Delta S_i^y S_j^y + S_i^z S_j^z\right] - h \sum_i S_i^z$$

QPT of disordered systems

Local density type approximations may be useful here.

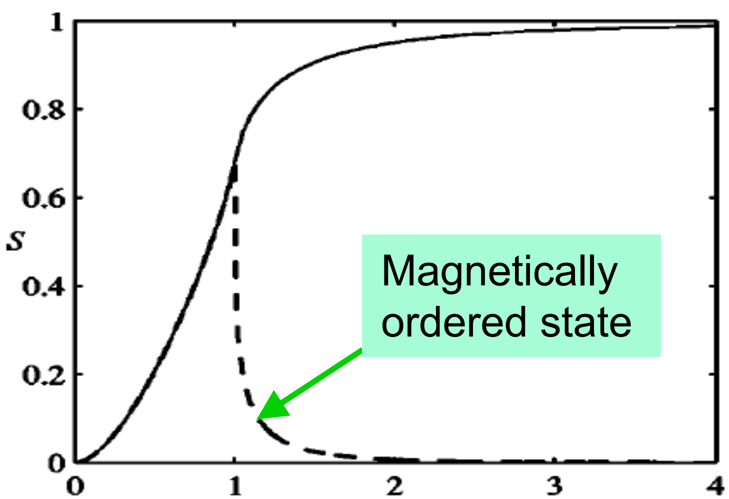
The approach remains to be explored.

Entanglement & QPT: Transverse field Ising chain

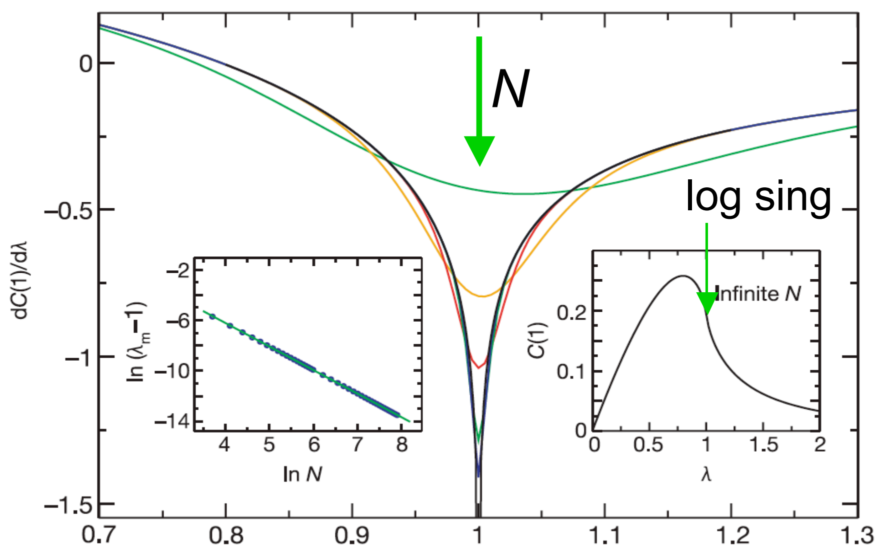
$$H = -J\left(\sum_i \sigma_i^x \sigma_{i+1}^x + \lambda \sum_i \sigma_i^z\right)$$

Bipartite entanglement entropy of one spin and the rest

Entanglement meas. of nearest neighbors - concurrence $C(\lambda)$ (Wootters, PRL 98)



$1 / \lambda$



$1 / \lambda$

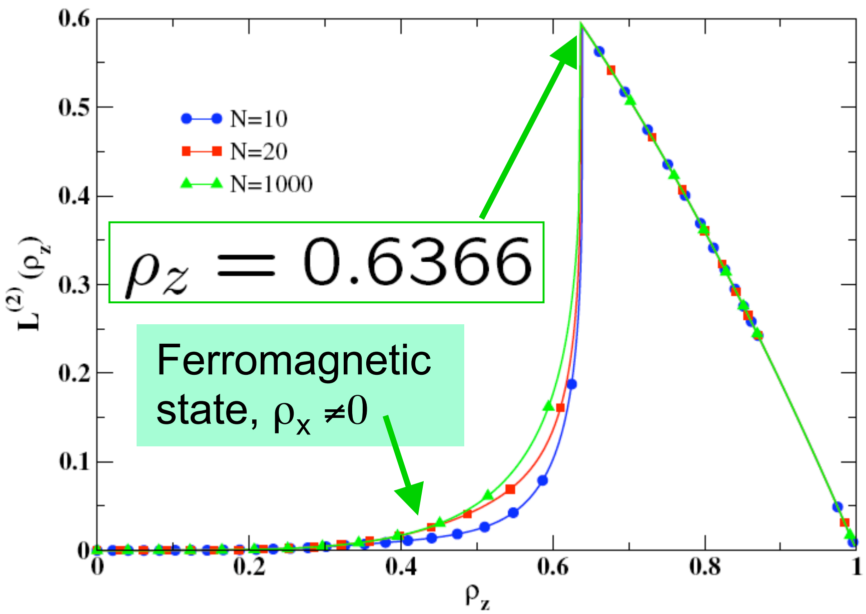
Osborne & Nielsen, PRA 66, 032110 (2002)

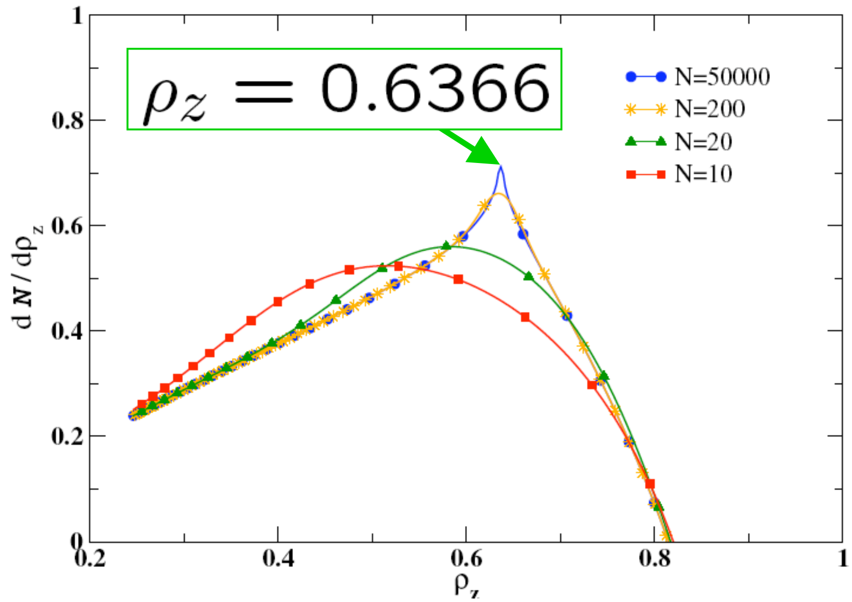
Osterloh, Amico, Falci & Fazio, Nature 416, 608 (2002)

Application of DFT to Transverse Field Ising Chain

Transverse magnetization as variable

$$\rho_z = \langle \psi | \sigma^z | \psi \rangle$$





Bipartite entanglement of one spin and the rest: Linear entropy

$$L_i^{(2)} = 1 - |\vec{\rho}_i|^2$$

Bloch vector

n.n. spins entanglement measure:

Negativity

$$\mathcal{N}(\rho) \equiv \frac{\|\rho^{T_A}\|_1 - 1}{2}$$

Sum of eigenvalue magnitudes

$$\langle i_A, j_B | \rho^{T_A} | k_A, \ell_B \rangle = \langle k_A, j_B | \rho | i_A, \ell_B \rangle$$

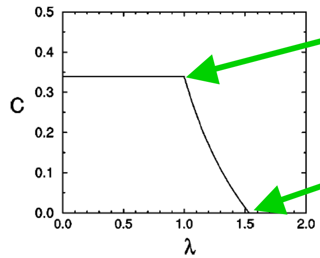
L J Sham 11/30/07

Caveats on Entanglement as Indicator of QPT

Non-analyticities which are not PT

MF Yang, PRA 71, 030302 (2005)

Concurrence $C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$ Wootters 98



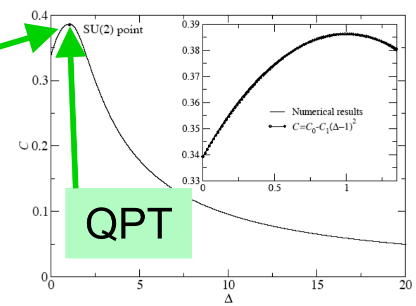
QPT

XX3 model

$$H = -\sum_{i=1}^{N} \left[\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \frac{\lambda}{2}(\sigma_{i-1}^x \sigma_i^z \sigma_{i+1}^y - \sigma_{i-1}^y \sigma_i^z \sigma_{i+1}^x) \right],$$

not QPT, non-analyticity from C

Subtler signals from entanglement



XXZ model

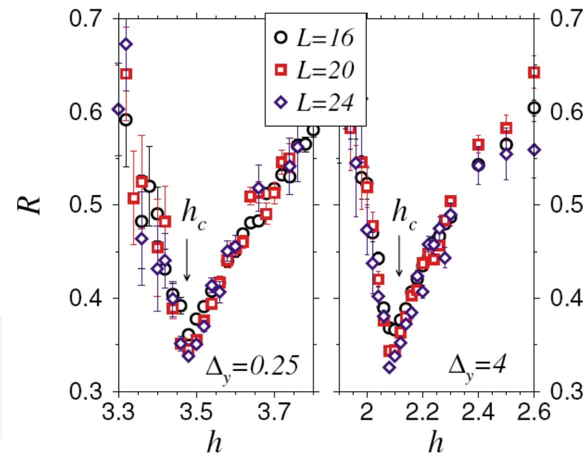
$$H(\Delta) = \sum_{l} [\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y + \Delta \sigma_l^z \sigma_{l+1}^z]$$

Competition between quantum fluctuation and order

Gu, Lin & Li, PRA 84, 042330 (2003)

Multi-spin entanglement

$$R = \frac{\text{(2-spin concur)}}{\text{(spin-rest ent)}}$$



Roscilde, Verrucchi, Fubini, Haas & Tognetti, PRL 94 (05)

Summary

- Quantum phase transition is driven by quantum fluctuations around a critical region of the field parameters of the Hamiltonian.
- Dominance of correlation over long distances is usually a measure of QPT.
- Entanglement in the critical region may be a quantum signal of QPT but ∃ CAVEATS. (A complete theory does not yet exist.)
- DFT: replace the functional dependence on the field parameters with the functional dependence on the corresponding "polarizations"