The Heisenberg Model

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Intrinsic Magnetic Moments of Electrons

$$\mu_s = -(e/m)\,\mathbf{S}.$$

- **S** is called *Spin*, with unit of $h/2\pi$.
- Electron: $S = 1/2$, $\mu_s = -\,1.0012\ \mu_B$;
- Proton: $S = 1/2$, $\mu_s = +\,0.0015\ \mu_B$;
- Neutron: $S = 1/2$, $\mu_s = -\,0.0010\ \mu_B$;

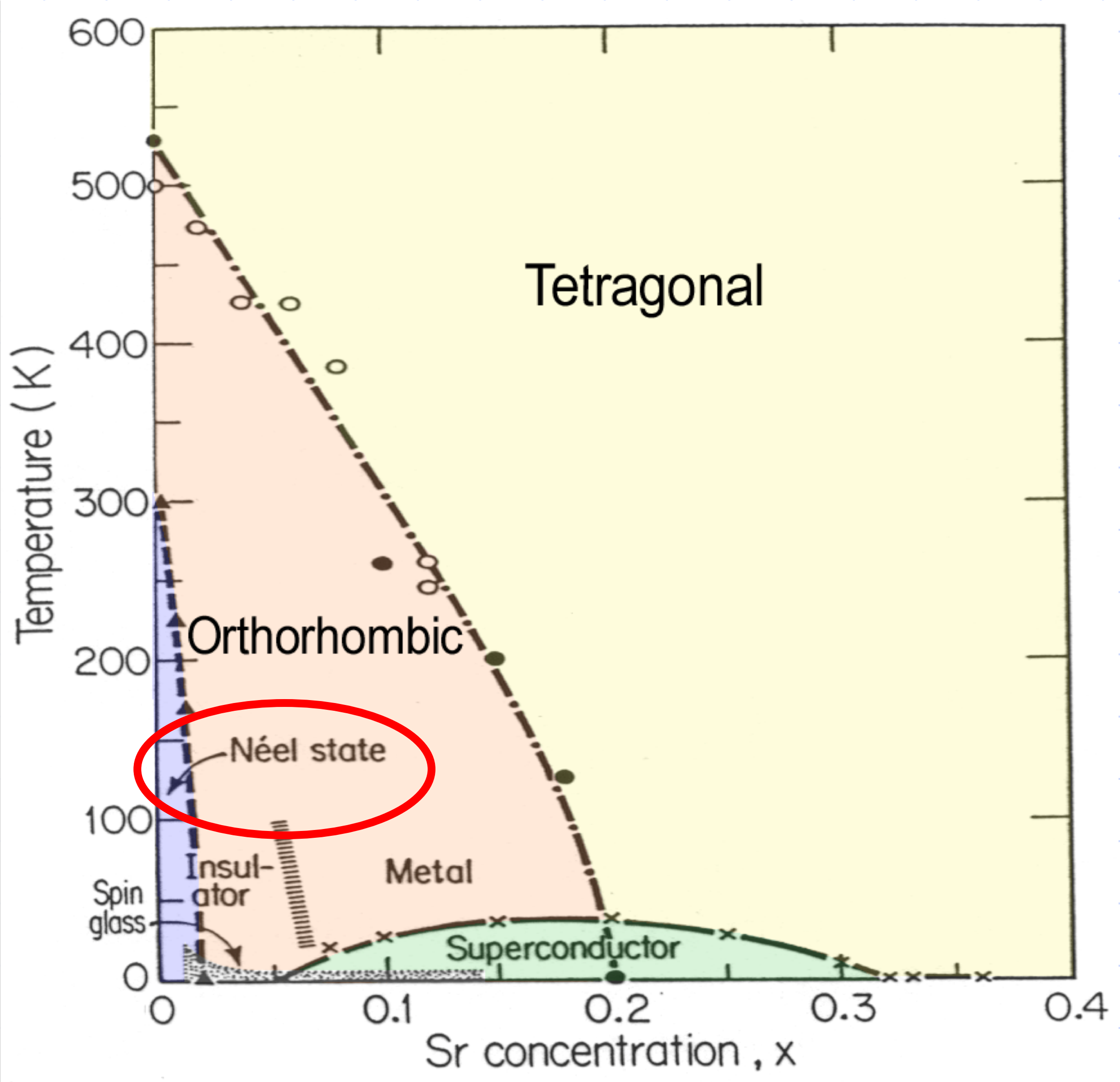
Magnetic Properties

- The magnetic properties of a material are determined by the total magnetic dipole moment of its atoms,

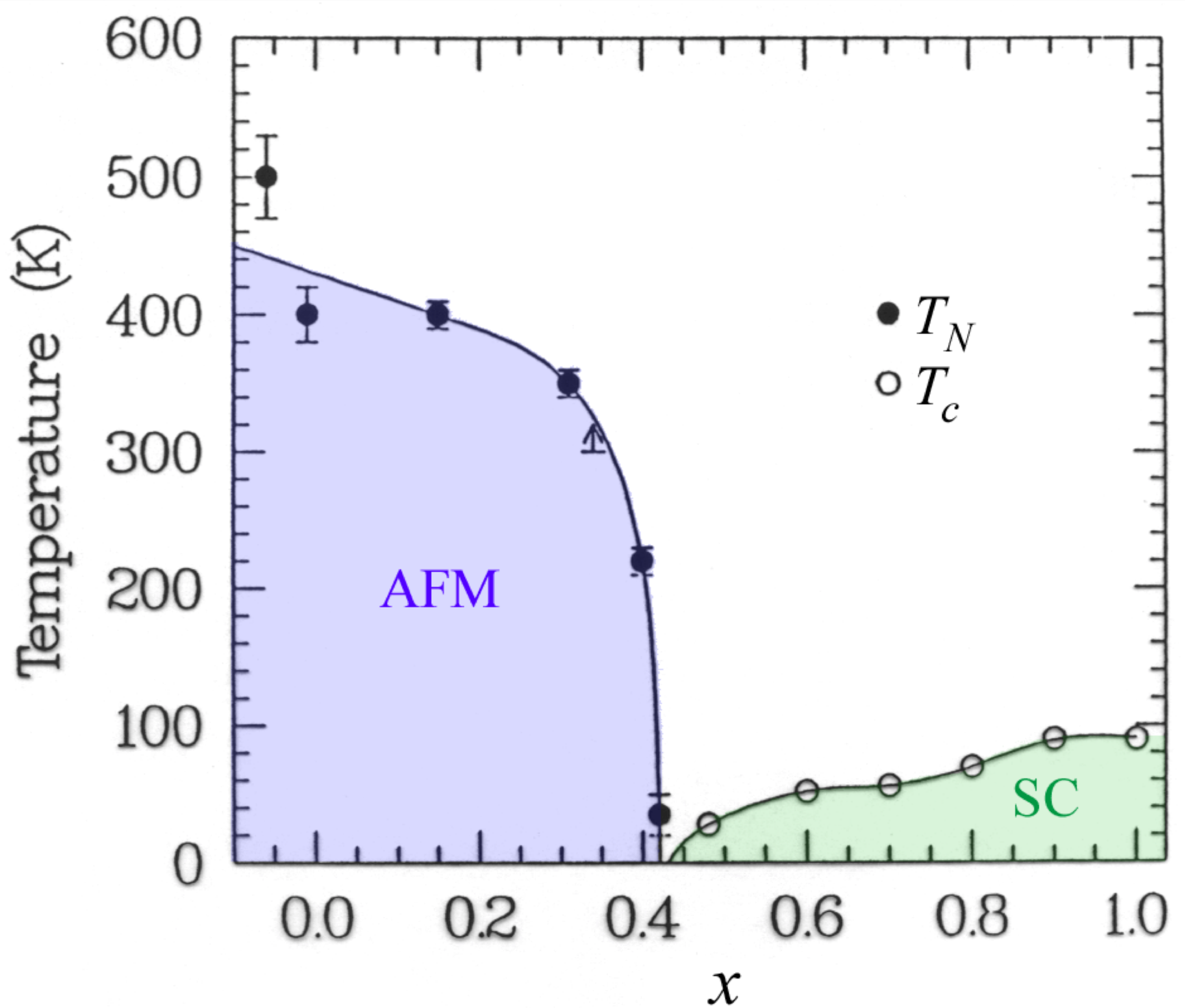
$$\mathbf{L}\ (= \Sigma_i\, \mathbf{l}_i) \qquad \textit{classical}$$
$$+$$
$$\mathbf{S}\ (= \Sigma_i\, \mathbf{s}_i) \qquad \textit{quantum mechanical}$$

- *The Spin part is more important.*

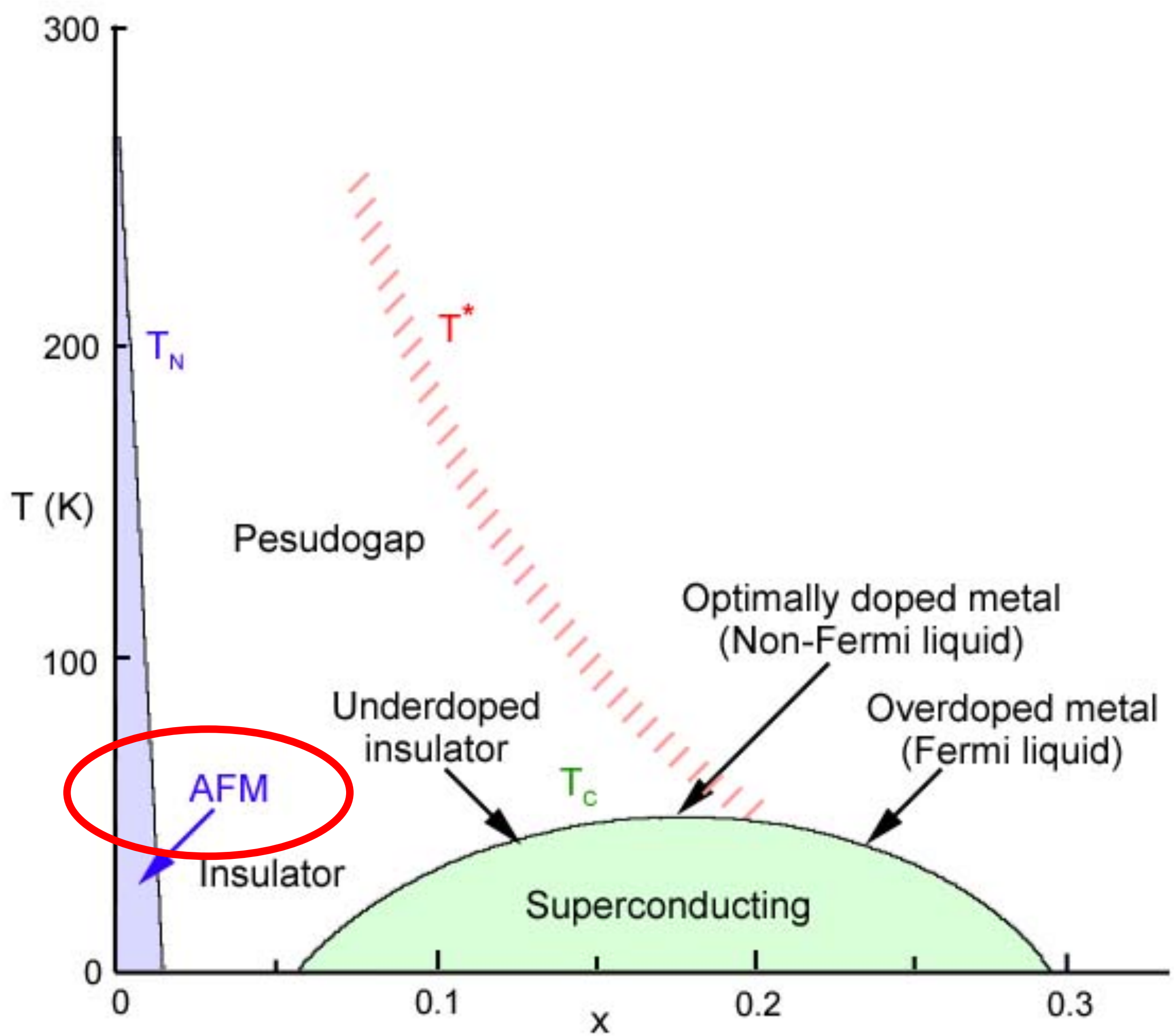
$La_{2-x}Sr_xCuO_4$ Phase Diagram



$YBa_2Cu_3O_{6+x}$ Phase Diagram



Generalized Phase Diagram Cond-mat/9802202



Issues

- AFM Long-Range Order at $x = 0$
- Dynamics of doped Mott-insulator
- Superconductivity
- …

Magnetic Properties of Undoped Compounds — Long-Range Antiferromagnetic Order

- Staggered magnetization m_s

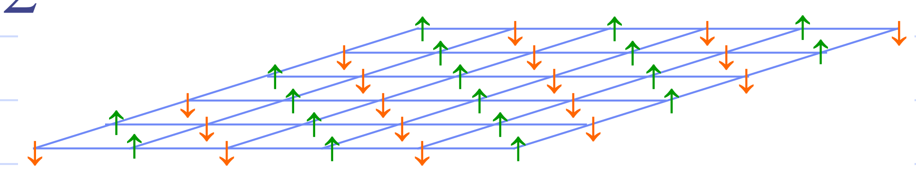
$$m^2 = \frac{1}{N^2}\sum \varepsilon_i \varepsilon_j \left\langle S_i^\alpha S_j^\alpha \right\rangle \quad \varepsilon_i = \begin{cases} 1 \\ -1 \end{cases}$$

Sublattice A

Sublattice B

$$m_s = \lim_{N\to\infty} m, \qquad m_s \neq 0 \;\Rightarrow\; \text{LRO}$$

- Neél ordering $m_s = 1/2$ (classical state)



- Quantum Fluctuation

$\mathbf{S}_i \cdot \mathbf{S}_j = S_i^z S_j^z$ Ising (**Neél**)

$+ \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$ Spin flip

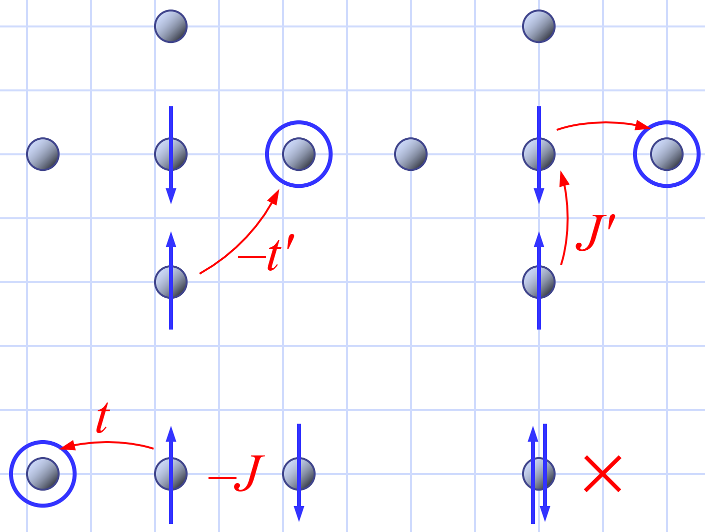
(Fluctuation)

Strong Coupling Limit ($U >> t$)

- Eliminate Double Occupied States
- 2nd order Degenerate Perturbation Theory (Schriffer-Wolff Transformation)

$$H_{SC} = H_{t\text{-}J} + -t' \sum_{\langle i,j,k\rangle,\sigma} \left(c^{\dagger}_{i,\sigma} n_{j,-\sigma} c_{k,\sigma} + H.c \right) + J' \sum_{\langle i,j,k\rangle,\sigma} \left(c^{\dagger}_{i,\sigma} c^{\dagger}_{j,-\sigma} c_{j,\sigma} c_{k,-\sigma} + H.c \right)$$

$$H_{t\text{-}J} = -t \sum_{\langle i,j\rangle,\sigma} \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + H.c \right) + \underbrace{J \sum_{\langle i,j\rangle} \left(\mathbf{S}_i \bullet \mathbf{S}_j - \tfrac{1}{4} n_i n_j \right)}_{\text{Heisenberg Model}}$$



- ½-Filled Band: AF Heisenberg Model
- $J = 4t^2/U$, $t' = J' = t^2/U$ (taken as free parameters)

Ground-state Properties of the Two-Dimensional Hubbard Model

Lin, PRB 44, 7151 (1991)

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 44, NUMBER 13 1 OCTOBER 1991-I

Ground-state properties of the two-dimensional Hubbard model

H. Q. Lin

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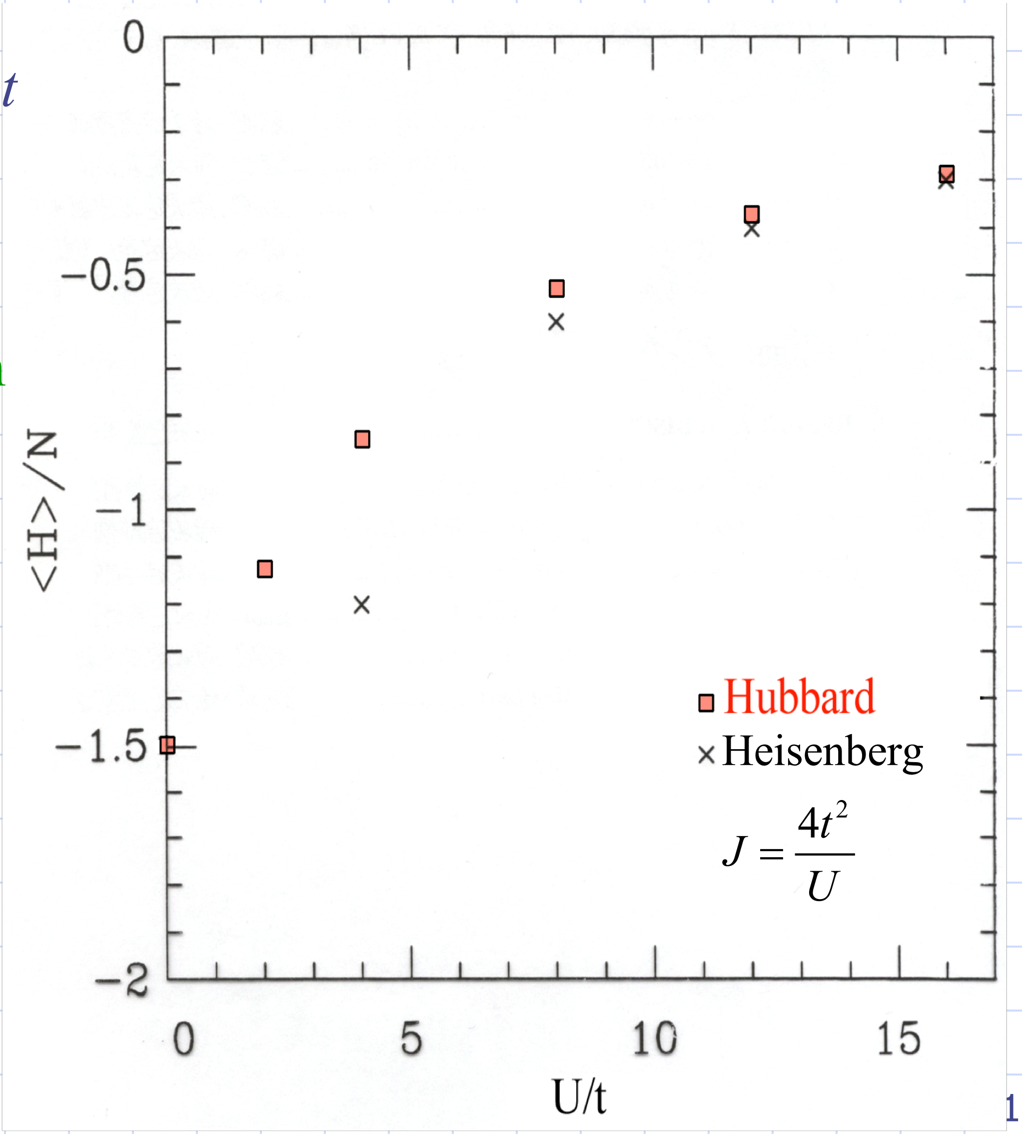
(Received 3 July 1991)

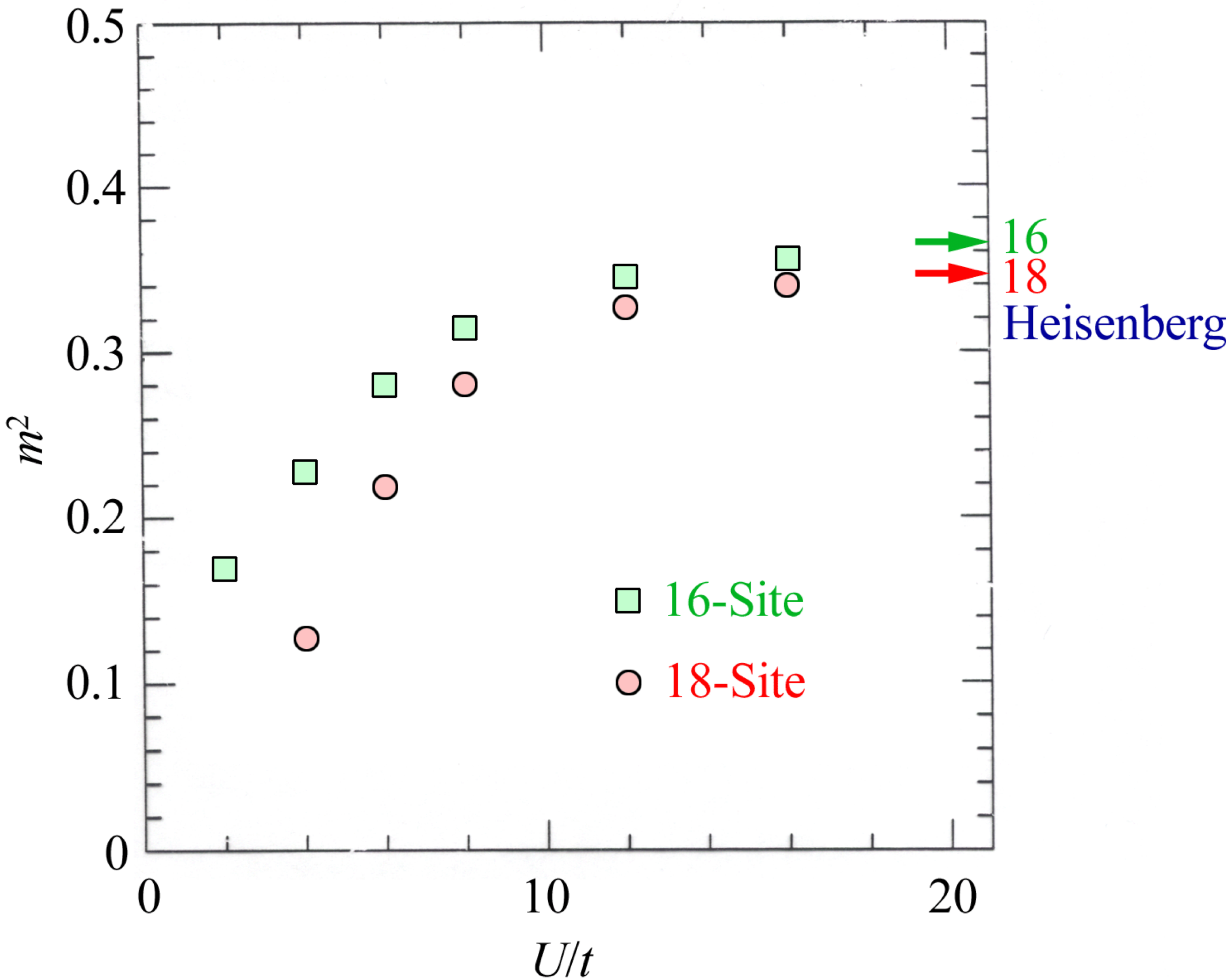
Using all appropriate symmetries for a two-dimensional square system, we have been able to diagonalize exactly the Hubbard Hamiltonian on the 4×4 and 18-site lattices. We calculate the ground-state energies, hole-hole interactions, and various correlation functions as functions of the Coulomb repulsion U and band filling, and compare the Hubbard-model results with those obtained from the t-J and strong-coupling models.

How strong is "strong"? (Hubbard model)

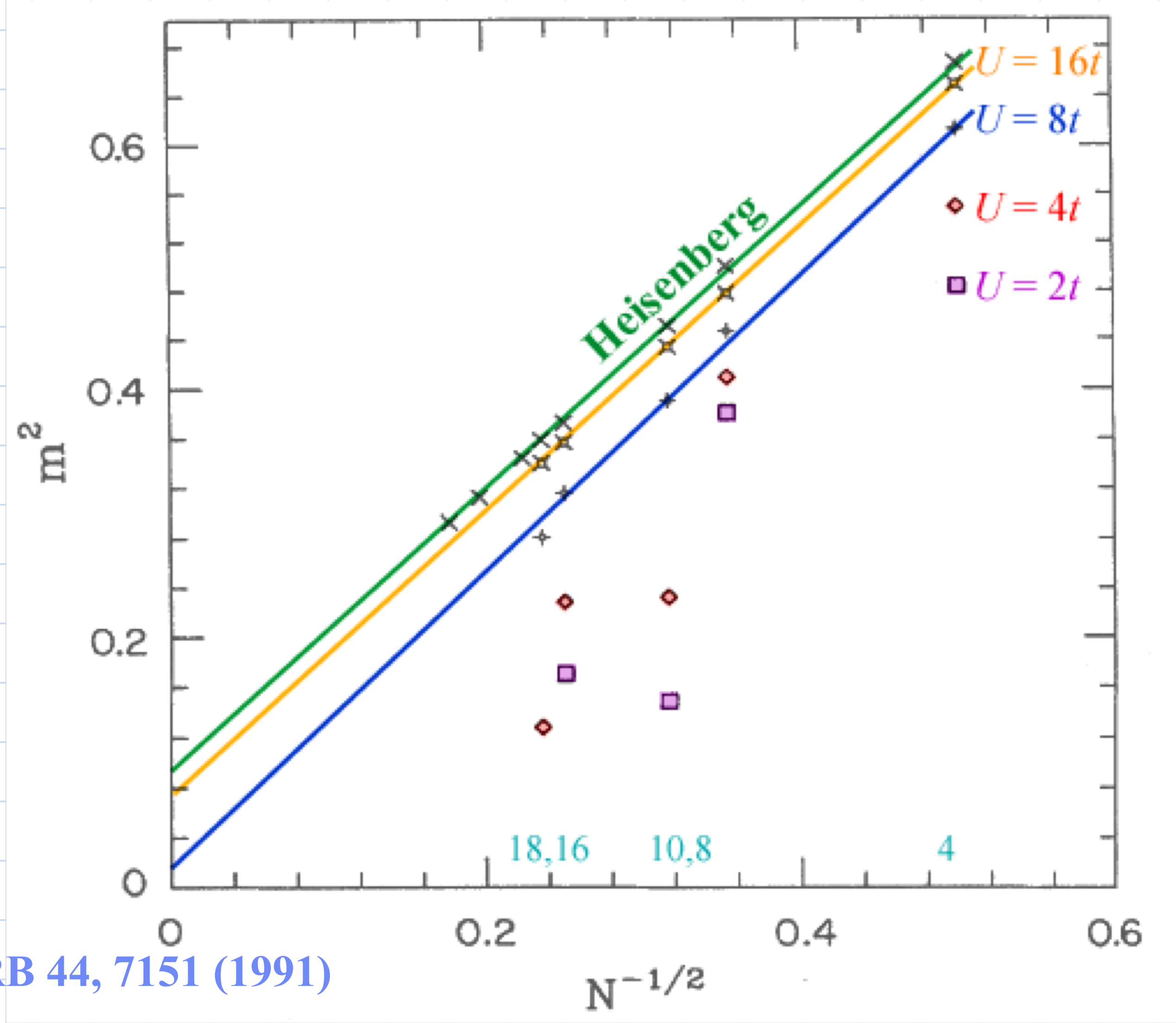
- $U > 8t$, 2D Hubbard $U \approx 6t$
- Away from ½-filled, U should be lager. O($1/U^2$) term in expansion
- $N = 4 \times 4$, ½-filled $\langle H \rangle / N$ vs U/t



Staggered magnetic moment in 2D Hubbard model, Half Filling - m^2 vs U/t



Staggered magnetic moment in 2D Hubbard model, Half Filling - m^2 vs $N^{-1/2}$



Lin, PRB 44, 7151 (1991)

XXZ Model Hamiltonian

$$H=\sum_{\langle i,j\rangle} J_x\left(S_i^x S_j^x + S_i^y S_j^y\right) + J_z S_i^z S_j^z = \sum_{\langle i,j\rangle} \frac{J_x}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) + J_z S_i^z S_j^z$$

where $\langle i, j\rangle$: Nearest-Neighbor Pair

S_i^α : Spin Operator on Site i

	J_z/J_x
FMH Model : $J_z = -J_x$	-1
XY Model : $J_z = 0$	0
AMH Model : $J_z = J_x \equiv J > 0$	1
Ising Model : $J_x = 0$	∞

Exact Diagonalization of the Quantum Spin Models

Lin, PRB 42, 6561 (1990)

PHYSICAL REVIEW B VOLUME 42, NUMBER 10 1 OCTOBER 1990

Exact diagonalization of quantum-spin models

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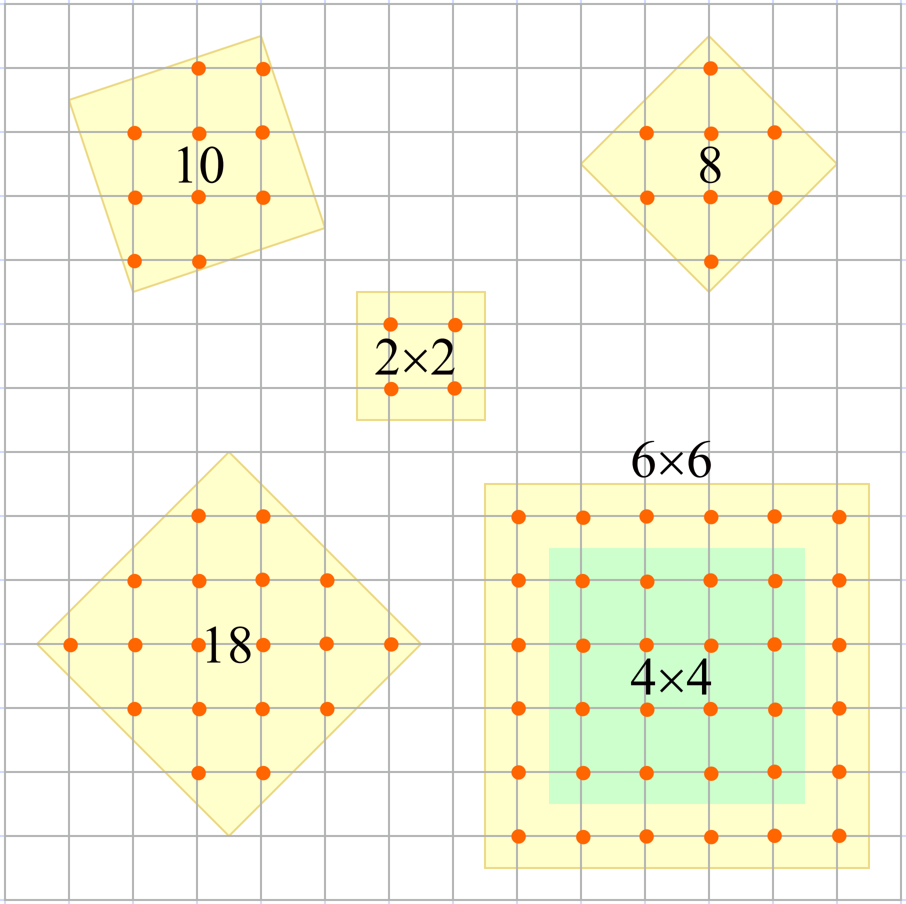
Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 12 April 1990)

We have developed a technique to replace hashing in implementing the Lanczös method for exact diagonalization of quantum-spin models that enables us to carry out numerical studies on substantially larger lattices than previously studied. We describe the algorithm in detail and present results for the ground-state energy, the first-excited-state energy, and the spin-spin correlations on various finite lattices for spins $S=\frac{1}{2}$, 1, $\frac{3}{2}$, and 2. Results for an infinite system are obtained by extrapolation. We also discuss the generalization of our method to other models.

Square Lattice (Oitma and Betts, 1978)

- $l^2 + m^2 = n$
- l, m, n are integers
- $l + m =$ even



Square Lattice (Oitma and Betts, 1978)

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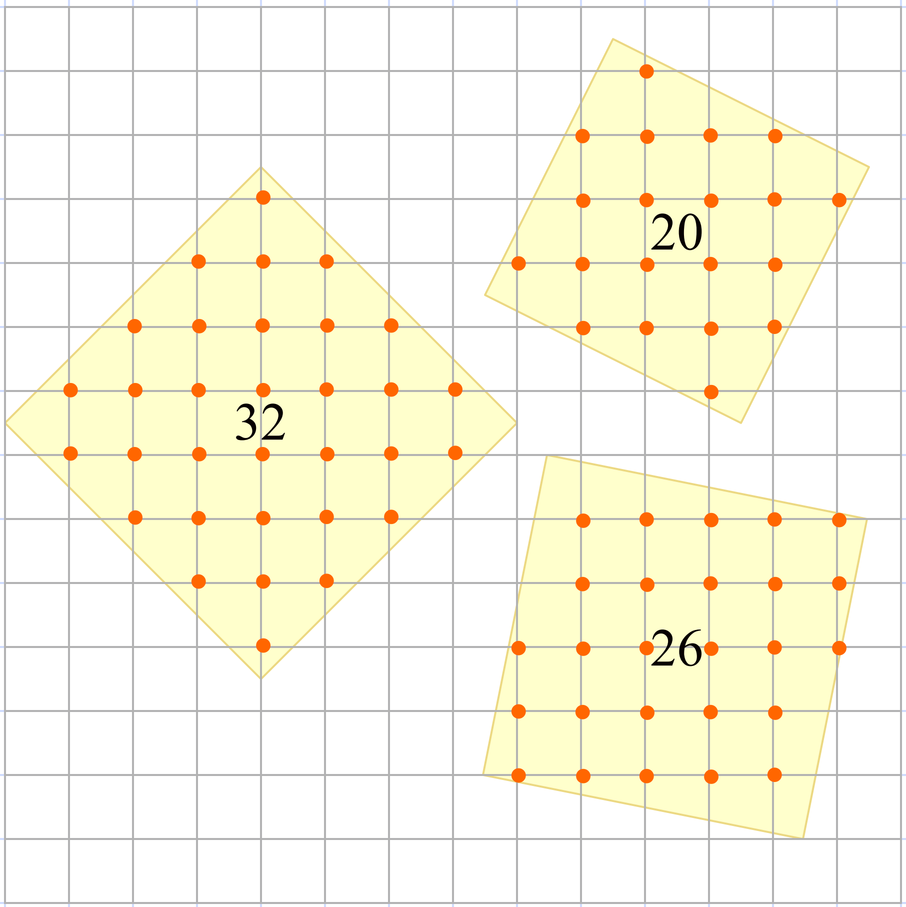

Exact Diagonalization and Quantum Monte Carlo Study of the spin-1/2 XXZ model on the square lattice

Lin, Flynn, Betts, PRB 64, 214411 (2001)

PHYSICAL REVIEW B, VOLUME 64, 214411

Exact diagonalization and quantum Monte Carlo study of the spin-$\frac{1}{2}$ XXZ model on the square lattice

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(Received 29 March 2001; published 8 November 2001)

The spin-$\frac{1}{2}$ XXZ model on an infinite square lattice at zero temperature has been studied and is presented here. Our methods using finite square lattices have been the exact diagonalization and quantum Monte Carlo methods. The physical properties estimated per lattice vertex include ground-state and first-excited-state energy, staggered magnetization, and susceptibility in the parallel and perpendicular directions, spin stiffness, and spin-wave velocity. In the XXZ model range from the Ising model to the Heisenberg model our estimates of physical properties compare very well with estimates by several other methods published in several other papers. In the XXZ range between the Heisenberg and XY models there is very little in the literature to compare with our finite lattice estimates of physical properties.

More Bipartite Square Lattice (ED Studies)

- **Old:**
  $N =$ 8, 10, 4×4, 18, 20, 26, 32, 6×6 (8 total)
- **New:**
  $N =$ 12, 16, 18, 22, 24 (4), 26, 28 (2), 30, 32, 34, 38 (15 additions)
- Topological bipartite imperfection, $I_B(N)$
- QMC: 16×16

Comparison of estimates of the energy per vertex, ε_0, and the staggered magnetization per vertex, m^+, of the $S = ½$ Heisenberg antiferromagnet on the infinite square lattice at $T = 0$

$-\varepsilon_0(\infty)$	$m^+(\infty)$	**Method**	**Reference**
0.6657(4)	–	Variational	[32] Liang, Doucet, Anderson
0.6638	–	Variational	[33] Hulse, Elser
0.66968	0.31	Coupled cluster	[34] Zeng, Farnell, Bishop
0.66934(3)	0.3075(25)	Quantum Monte Carlo	[35, 36] Runge
0.669437(5)	0.3070(3)	Series expansion QMC	[37] Sandvik
0.669442(26)	0.3077(4)	Green function MC	[38] Buonaura, Sorella
0.66999	0.3069	Third order spin wave	[39] Hamer, Zheng
0.66949	0.30686(10)	Fourth order spin wave	[40] Zheng, Hamer
0.668(1)	0.33(3)	t expansion	[41] Zheng, Oitmaa, Hamer
0.6696(3)	0.303(8)	Series expansion	[42] Singh
0.6693(1)	0.307(1)	Series expansion	[43] Wiese, Ying
0.669(1)	0.325	ED on finite lattices	[19] Schaltz, Ziman, Poilblanc
0.6513(8)	0.20(1)	Ditto	[15] Horsch, von der Linden
0.66960(13)	**0.303(2)**	**Ditto**	**Present estimates**

Lin, Flynn, Betts, PRB 64, 214411 (2001), and references therein

Exact Diagonalization (ED)

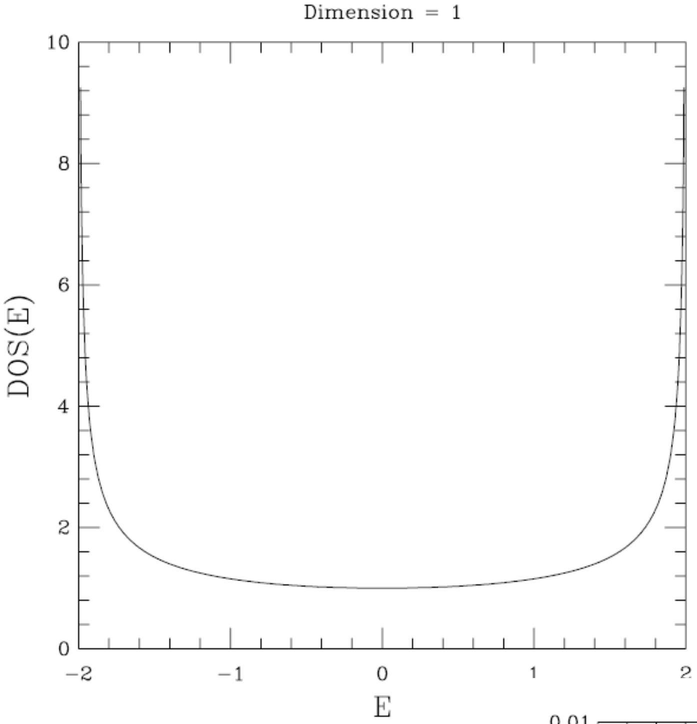
- Exact solution on finite lattice
- Gain insights about correlations
- Flexibility (BC, interactions, etc)
- Check on approximations and simulations
- Finite size scaling scheme is desired
- Usually prefer short-range interactions

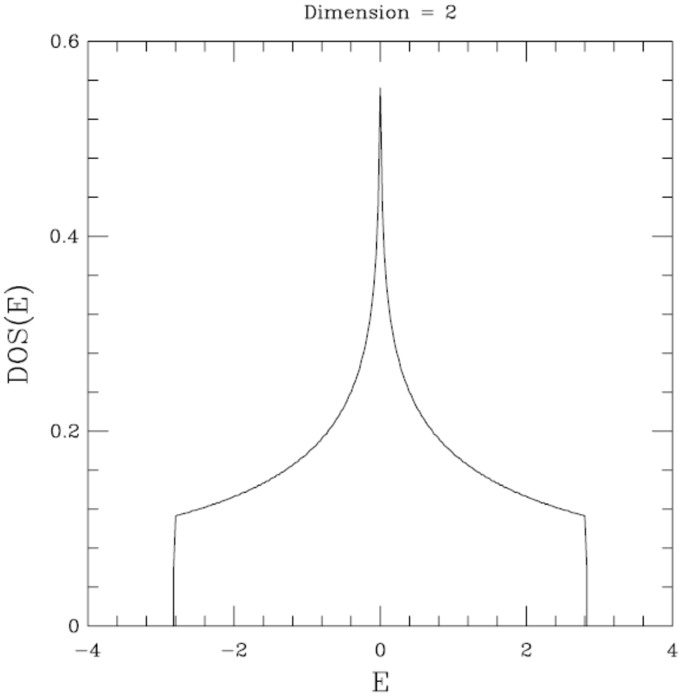
- **See lecture note on ED**

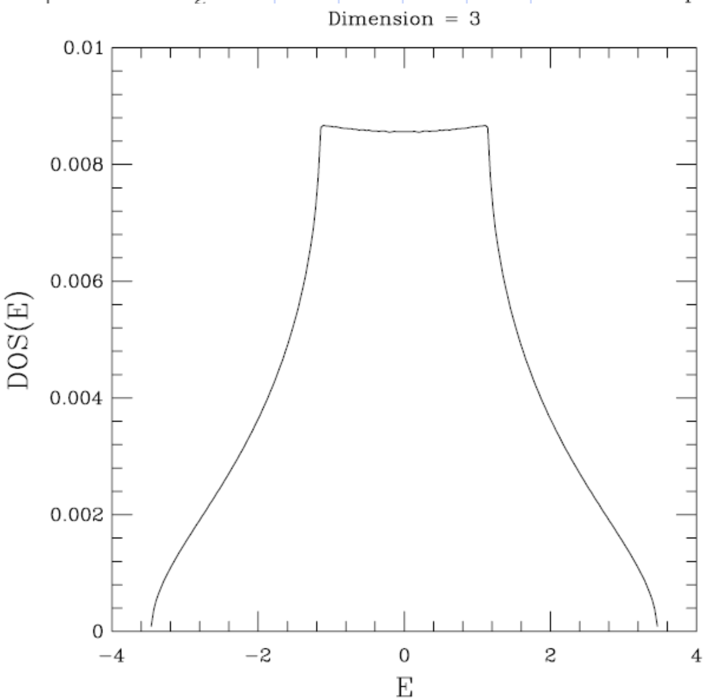
Dimensionality D

- Affects physical properties greatly
- $D = 0$, most models could be solved analytically
- $D = 1$, many models could be solved analytically
- $D = \infty$, most models could be solved
- $D \geqq 4$, mean-field solution acceptable
- $D = 3$, some approximation schemes work
- $D = 2$, the most difficult

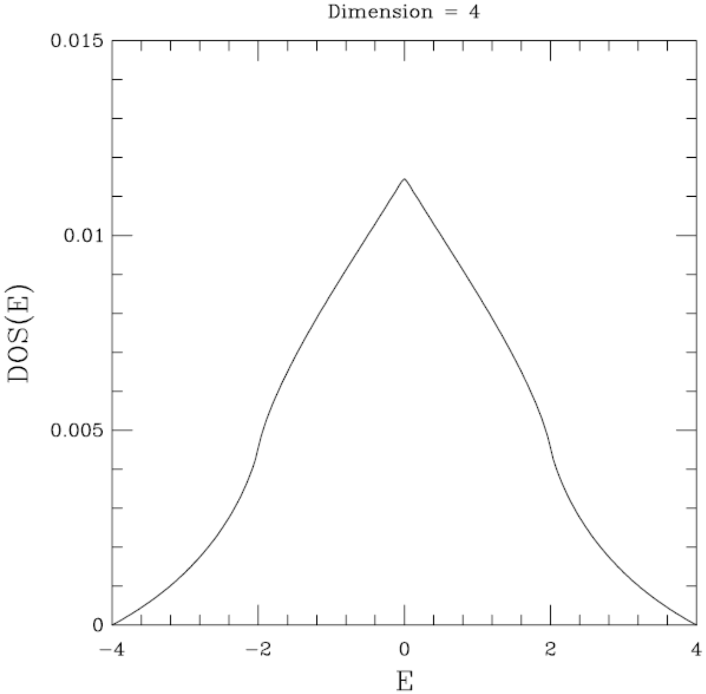
D=1,2,3

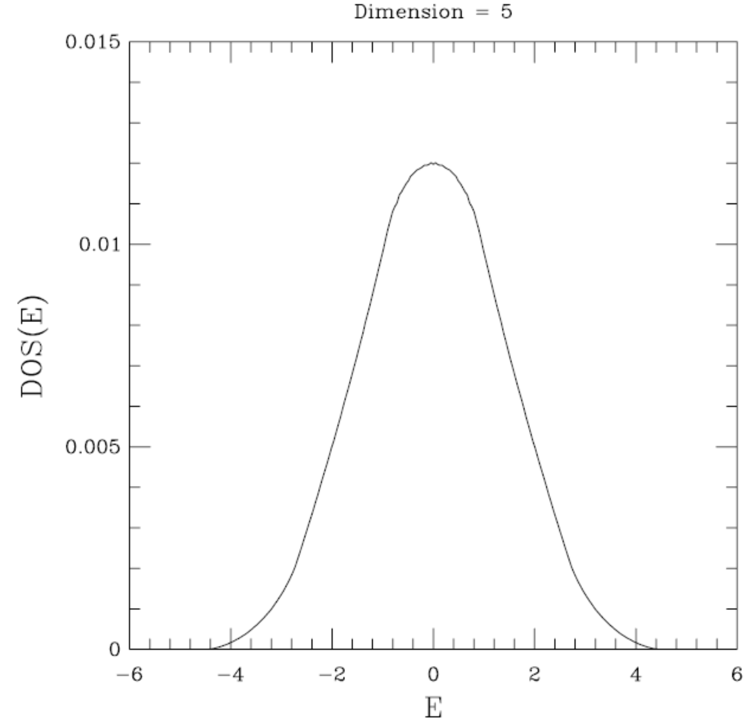

Dimension = 1
DOS(E)
E
10
8
6
4
2
0
−2
−1
0
1
2

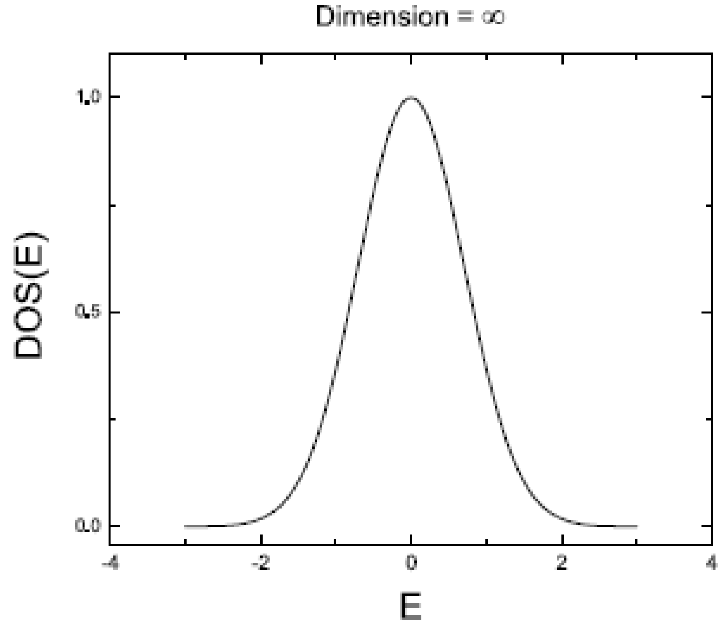

Dimension = 2
DOS(E)
E
0.6
0.4
0.2
0
−4
−2
0
2
4


Dimension = 3
DOS(E)
E
0.01
0.008
0.006
0.004
0.002
0
−4
−2
0
2
4

D=4,5,∞


Dimension = 4
DOS(E)
E
0.015
0.01
0.005
0
−4
−2
0
2
4


Dimension = 5
DOS(E)
E
0.015
0.01
0.005
0
−6
−4
−2
0
2
4
6


Dimension = ∞
DOS(E)
E
1.0
0.5
0.0
-4
-2
0
2
4

THE PHASE DIAGRAM OF THE ONE-DIMENSIONAL EXTENDED HUBBARD MODEL

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[3] Theoretical Division, MS B 262, Los Alamos National Laboratory
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ABSTRACT

For a wide range of its three parameters – the Coulomb interactions U and V and the band filling ρ – we obtain the phase diagram of one-dimensional. "conventional" extended Hubbard model by combining previously known weak-coupling results with strong coupling perturbation theory, quantum Monte Carlo (QMC), and exact diagonalization) simulations. Our results establish the existence of a variety of phases, including several not predicted by weak coupling arguments. We delineate, for all ρ, the regions of the U, V parameter plane in which the model exhibits the "Luttinger Liquid" behavior expected for a strongly correlated, one-dimensional metal. In other regions, we establish the nature of the dominant fluctuations and, if relevant, the broken symmetry ground states. We evaluate the charge-charge, spin-spin, and superconducting pairing susceptibilities and correlation functions and calculate the charge correlation exponent, K_ρ. Our results are generally consistent with, but substantially extend, previous analyses based on QMC, exact diagonalization, and renormalization group studies.

The Hubbard Model, Edited by D. Baeriswyl
et al., Plenum Press, New York, 1995

Solving the Hubbard Model

- Mean-field approximation, Hartree-Fock
- Why mean-field?
- $n_{i\uparrow} n_{i\downarrow} \rightarrow \; <n_{i\uparrow}> n_{i\downarrow} + n_{i\uparrow} <n_{i\downarrow}> - <n_{i\uparrow}><n_{i\downarrow}>$
- Many-body → one-body
- Usually not good in low dimensions
- Exact in ∞ dimension

  (see notes on Hartree-Fock approach)

Mean-Field Approach

PHYSICAL REVIEW VOLUME 142, NUMBER 2 FEBRUARY 1966

Stability Theory of the Magnetic Phases for a Simple Model of the Transition Metals*†

DAVID R. PENN‡
Department of Physics and Institute for the Study of Metals, University of Chicago, Chicago, Illinois

(Received 4 August 1965)

A semiquantitative explanation of the observed distribution of magnetism in the transition metals and alloys is made based on a highly simplified quasiparticle band model. It depends on only two parameters, the valence (number of d electrons) of the metal and the ratio of quasiparticle interaction strength to bandwidth, C_0/E''. The quantity C_0/E'' increases with valence and also increases as one goes from the $5d$ transition metals to the $3d$ transition metals. Ferromagnetism is found to be most likely for those metals with large C_0/E'' and a valence well away from five. Antiferromagnetism is found to occur for a valence of around five, as do the more complex states such as the ferrimagnetic and spiral-spin-density-wave states, which are explicitly described. It is suggested that the peak in the specific heat of the transition-metal alloys that occurs as one alloys across the $3d$ transition series is closely related to changes in the band structure caused by ordering, at least for the Cr-Mn system.

Mean-Field Approach

PHYSICAL REVIEW B VOLUME 31, NUMBER 7 1 APRIL 1985

Two-dimensional Hubbard model: Numerical simulation study

J. E. Hirsch

Department of Physics, University of California, San Diego, La Jolla, California 92093

(Received 1 October 1984)

We have studied the two-dimensional Hubbard model on a square lattice with nearest-neighbor hopping. We first discuss the properties of the model within the mean-field approximation: Because of the form of the band structure, some peculiar features are found. We then discuss the simulation algorithm used and compare simulation results with exact results for 6-site chains to test the reliability of the approach. We present results for thermodynamic properties and correlation functions for lattices up to 8×8 in spatial size. The system is found to be an antiferromagnetic insulator for all values of the coupling constant at zero temperature in the half-filled-band case, but the long-range order is much smaller than predicted by mean-field theory. We perform a finite-size-scaling analysis to determine the character of the transition at zero coupling. For non-half-filled-band cases, our results suggest that the system is always paramagnetic, in contradiction with Hartree-Fock predictions. The system does not show tendency to ferromagnetism nor triplet superconductivity in the parameter range studied. We also discuss some properties of the attractive Hubbard model in the half-filled-band case.

Mean-Field Approach

PHYSICAL REVIEW B VOLUME 35, NUMBER 7 1 MARCH 1987

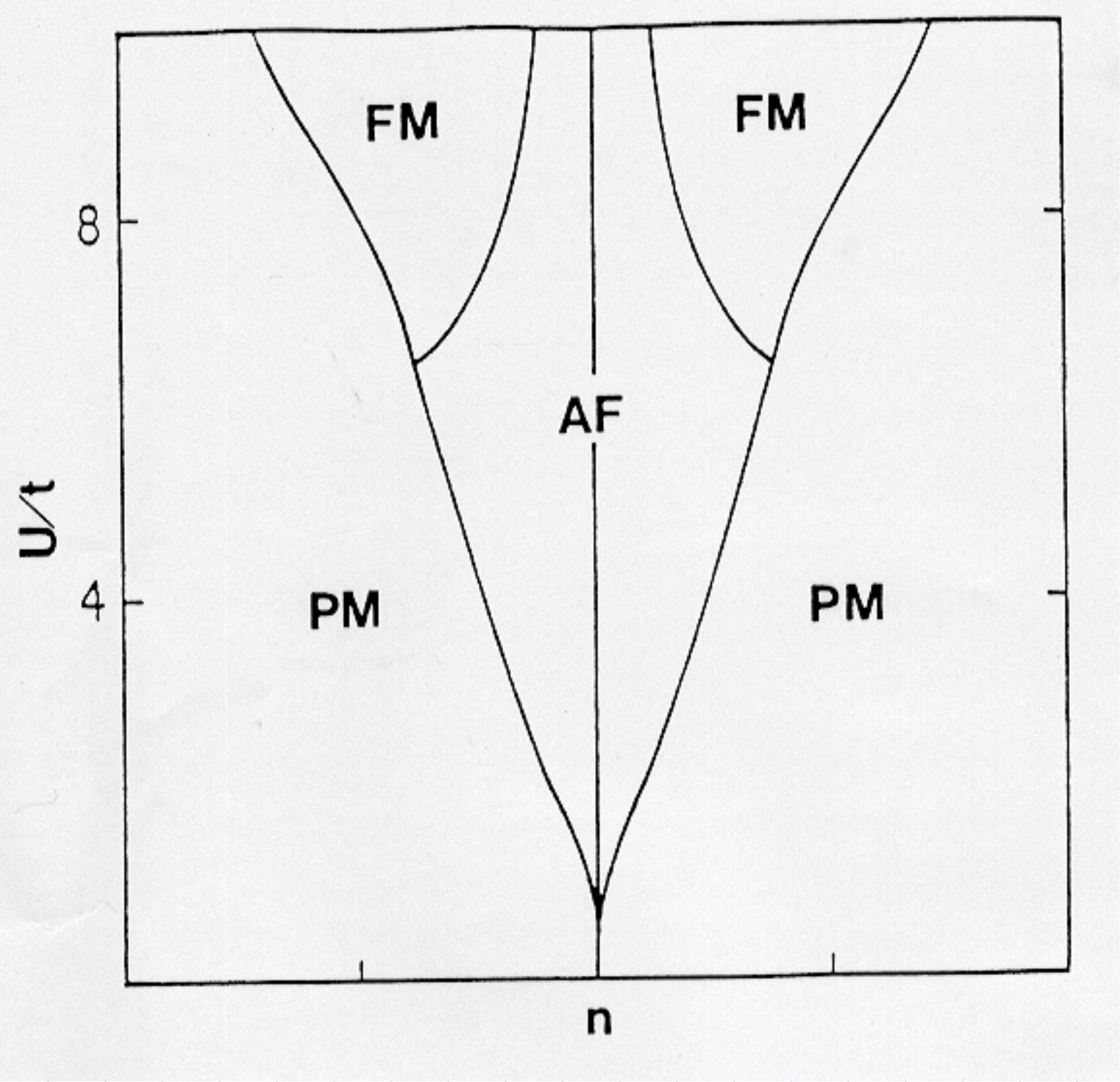
Two-dimensional Hubbard model with nearest- and next-nearest-neighbor hopping

H. Q. Lin and J. E. Hirsch
Department of Physics, University of California, San Diego, La Jolla, California 92093

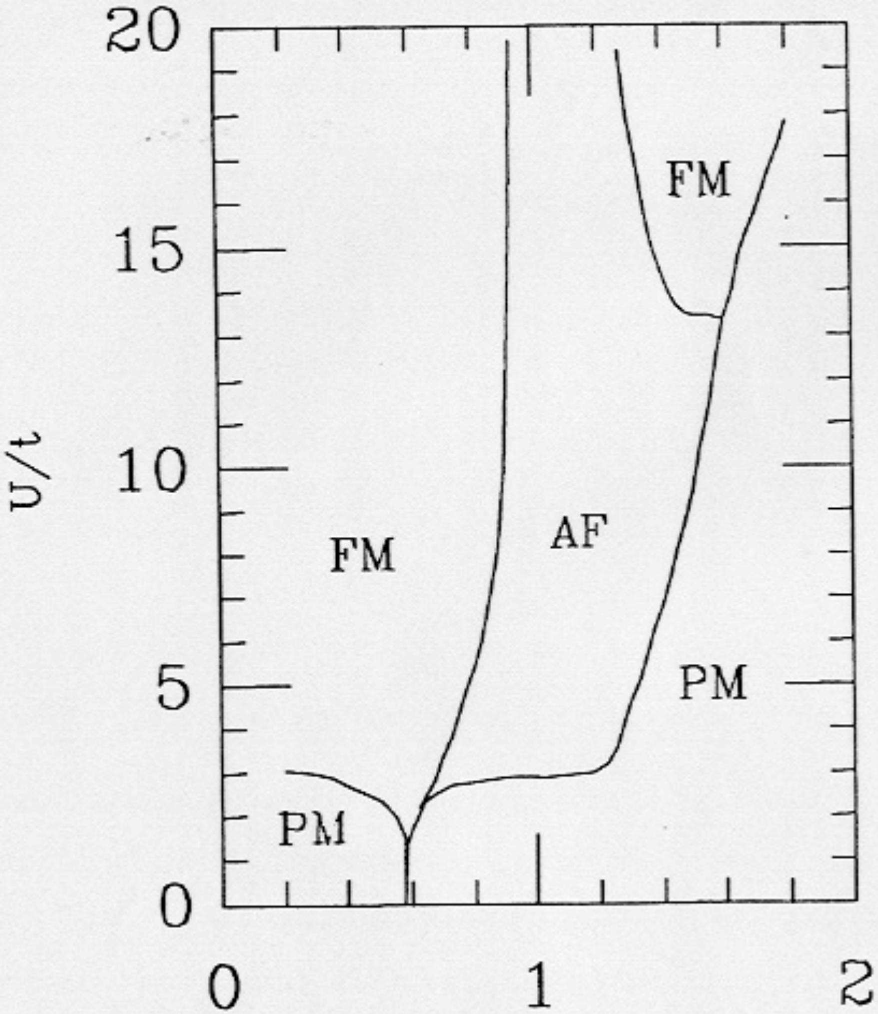
(Received 19 May 1986)

We study the magnetic properties of the two-dimensional Hubbard model with nearest-neighbor (t) and next-nearest-neighbor (t_2) hopping and on-site repulsion U. We first calculate the mean-field phase diagram as a function of band filling and U. Because of the Van Hove singularity in the density of states, we find a ferromagnetic phase extending to zero U for certain band filling. For the half-filled band case, antiferromagnetism sets in at a finite value of U if $t_2 \neq 0$. We study the behavior of spin-spin correlation functions for small lattices of up to $N=64$ atoms using Monte Carlo simulations, as well as exact diagonalization for $N=4$. Our results show enhanced ferromagnetic correlations in some regions, but apparently no ferromagnetic long-range order. In the half-filled case, our numerical results are consistent with a nonzero critical U. For a non-half-filled band our results suggest that there is no long-range order.

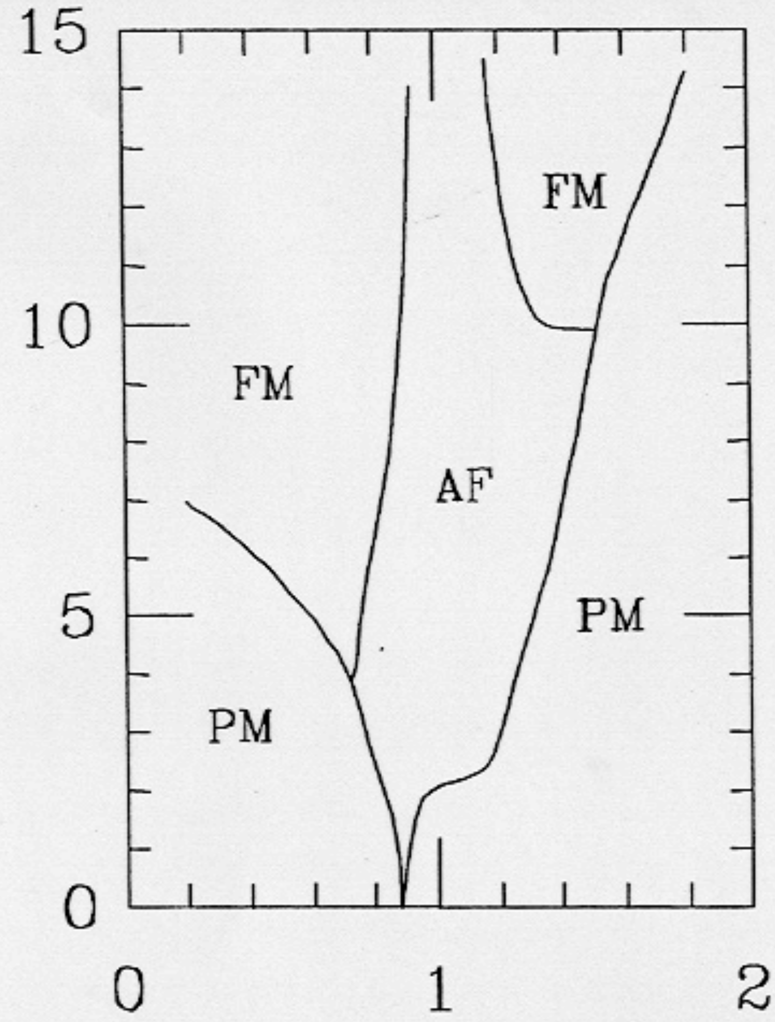
HF Phase Diagram (*t*-*U* model)



HF Phase Diagram (t-t_2-U model)



$t_2 = 0.2$



$t_2 = 0.4$

Mean-Field Approach – Slave Particle

- Perform canonical transformation
  - $c_{i\sigma} \longrightarrow f_i^\dagger \sigma_i$, f defines hole, $\boldsymbol{\sigma}$ defines spin
  - decouple spin and charge degrees of freedom
- Do mean-field on charge or spin operator
- There are other similar schemes

Solving Many-Body Problem

- Green's Function Decoupling
  (by Hubbard and others)

$$G_\sigma(\mathbf{k},\omega) = \frac{1}{\omega - (\epsilon(\mathbf{k}) - \mu) - \Sigma_\sigma^{atom}(\omega)}$$

$$\Sigma_\sigma^{atom}(\omega) = U n_{-\sigma} + U^2 \frac{n_{-\sigma}(1 - n_{-\sigma})}{\omega + \mu - U(1 - n_{-\sigma})}$$

- Perturbation Theory
  Small/Large t/U, slow converge
  Most interested region: $U \sim W = 2Dt$

Solving Many-Body Problem

- Path Integral Approach
  - Saddle point approximation plus fluctuations
  - Coherent Potential Approximation (CPA)
- Field Theory Approach: bosonization, etc.
- Variation Wave Functions: Gutzwiller, etc.
- …