Variational Monte Carlo Method for Fermions

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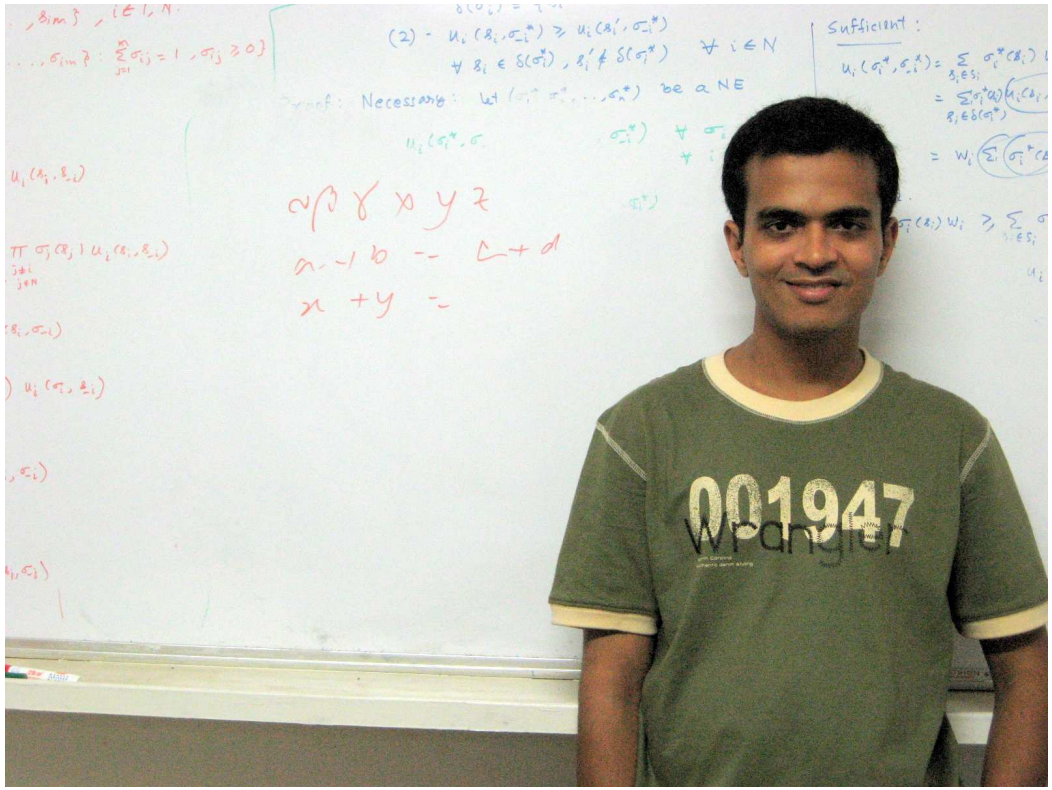
Acknowledgements



Sandeep Pathak

- Department of Science and Technology

Plan of the Lectures on Variational Monte Carlo Method

- Motivation, Overview and Key Ideas
- Details of VMC
- Application to Superconductivity

The Strongly Correlated Panorama...

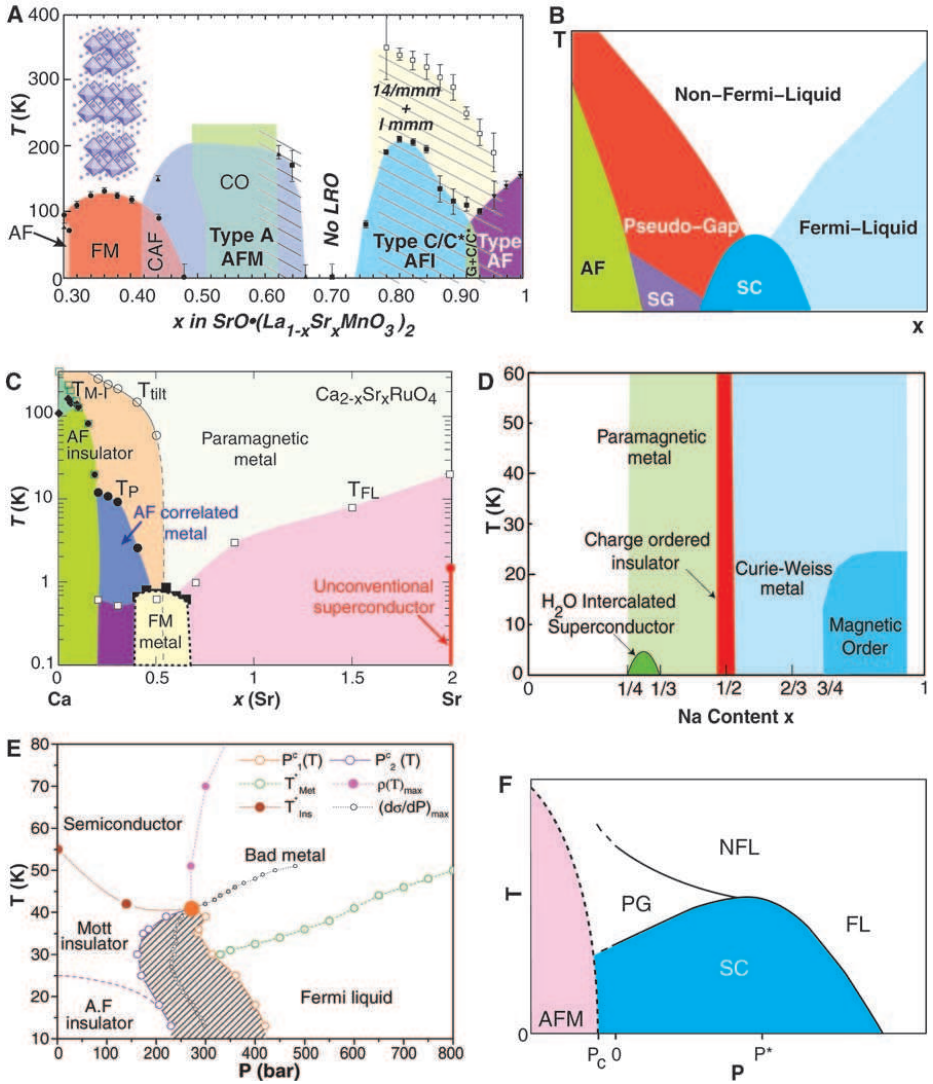
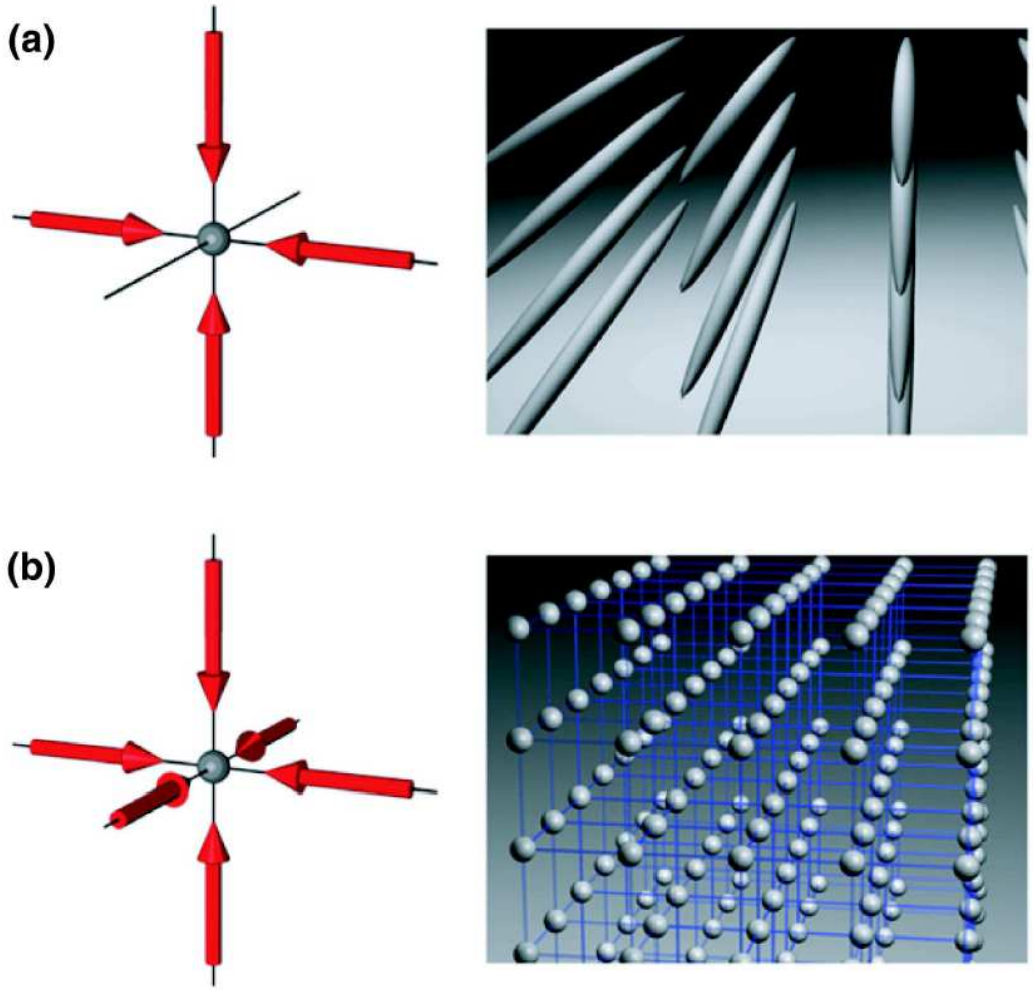


Fig. 1. Phase diagrams of representative materials of the strongly correlated electron family (notations are standard and details can be found in the original references). **(A)** Temperature versus hole density phase diagram of bilayer manganites (*74*), including several types of antiferromagnetic (AF) phases, a ferromagnetic (FM) phase, and even a globally disordered region at $x = 0.75$. **(B)** Generic phase diagram for HTSC. SG stands for spin glass. **(C)** Phase diagram of single layered ruthenates (*75*, *76*), evolving from a superconducting (SC) state at $x = 2$ to an AF insulator at $x = 0$ (x controls the bandwidth rather than the carrier density). Ruthenates are believed to be clean metals at least at large x, thus providing a family of oxides where competition and complexity can be studied with less quenched disorder than in Mn oxides. **(D)** Phase diagram of Co oxides (*77*), with SC, charge-ordered (CO), and magnetic regimes. **(E)** Phase diagram of the organic κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl salt (*57*). The hatched region denotes the coexistence of metal and insulator phases. **(F)** Schematic phase diagram of the Ce-based heavy fermion materials (*51*).

(Dagotto, *Science*, (2005))

...and now, Cold Atom Quantum Simulators



(Bloch et al., *RMP*, (2009))

- Hamiltonian...for here, or to go?

The Strategy

- Identify "key degrees of freedom" of the system of interest
- Identify the key interactions
- Write a Hamiltonian (eg. tJ-model)...reduce the problem to a model
- "Solve" the Hamiltonian
- ....
- Nature(Science)/Nature Physics/PRL/PRB...

"Solvers"

- Mean Field Theories (MFT)
- Slave Particle Theories (and associated MFTs)
- Dynamical Mean Field Theories (DMFT)
- Exact Diagonalization
- Quantum Monte Carlo Methods (eg. Determinental)
- Variational Monte Carlo (VMC)
- ...
- AdS/CFT

Great Expectations

Prerequisites

- Graduate quantum mechanics including "second quantization"
- Ideas of "Mean Field Theory"
- Some familiarity with "classical" superconductivity

At the end of the lectures, you can/will have

- Understood concepts of VMC
- Know-how to write your own code
- A free code (`pedestrianVMC`)
- Seen examples of VMC in strongly correlated systems

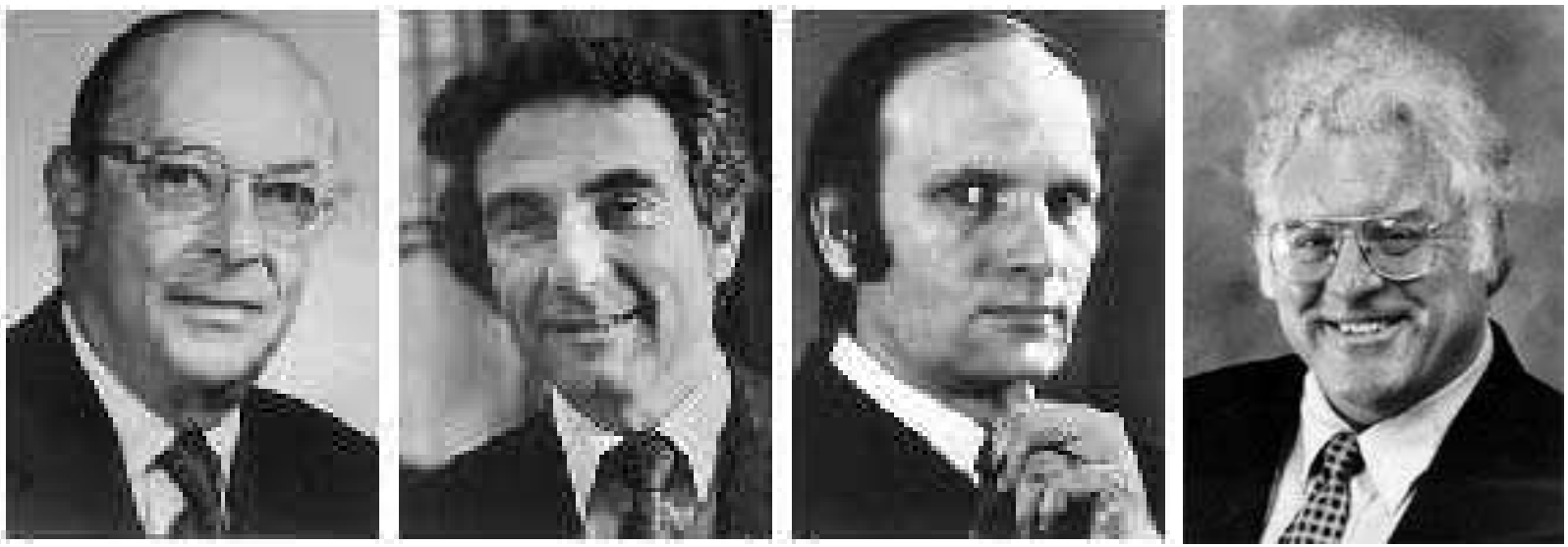
References

- NATO Series Lecture Notes by Nightingale, Umrigar, see `http://www.phys.uri.edu/~nigh/QMC-NATO/webpage/abstracts/lectures.html`
- Morningstar, `hep-lat/070202`
- Ceperley, Chester and Kalos, *PRB* **17**, 3081 (1977)

VMC in a Nutshell

- Strategy to study ground (and some special excited) state(s)
- "Guess" the ground state
- Use Schrödinger's variational principle to optimize the ground state
- Calculate observables of interest with the optimal state
- ...

Hall of Fame



Bardeen, Cooper, Schrieffer Laughlin

Quote/Question from A2Z, Plain Vanilla *JPCM* (2004)

The philosophy of this method (`VMC`)is analogous to that used by BCS for superconductivity, and by Laughlin for the fractional quantum Hall effect: simply guess a wavefunction. Is there any better way to solve a non-perturbative many-body problem?

Variational Principle

- Eigenstates of the Hamiltonian satisfy

$$H|\Psi\rangle = E|\Psi\rangle$$

  where E is the energy eigenvalue
- Alternate way of stating this
  - Define an "energy functional" for any given state $|\Phi\rangle$

$$E[\Phi] = \langle\Phi|H|\Phi\rangle$$

  - Among all states $|\Phi\rangle$ that satisfy $\langle\Phi|\Phi\rangle = 1$, those that extremize $E[\Phi]$ are eigenstates of H Exercise: Prove this!
  - The state(s) that minimises(minimise) $E[\Phi]$ is(are) the ground state(s)

Variational Principle in Action...A Simple Example

- Ground state H_2^+ molecule with a given nuclear separation
- "Guess" the wave function (linear combination of atomic orbitals)

$$|\psi\rangle = a|1\rangle + b|2\rangle$$

  where $|1, 2\rangle$ are atomic orbitals centered around protons 1 and 2
- Find energy function (taking everything real)

$$E(a, b) = H_{11}a^2 + 2H_{12}ab + H_{22}b^2$$

  (symbols have obvious meaning)
- Minimize (with appropriate constraints) to find $|\psi\rangle_g = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ (for $H_{12} < 0$) Question: Is this the *actual* ground state?
- Example shows key ideas (*and limitations*) of the variational approach!

Variational Approach in Many Body Physics

- Guess the ground state wavefunction $|\Psi\rangle$
- $|\Psi\rangle$ depends on some variational parameters $\alpha_1, \alpha_2 ...$ which "contain the physics" of the wavefunction
  - Example,

$$|BCS\rangle = \left[\prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)\right]|0\rangle$$

  u_k, v_k are the "α_is"
- In general, α_is are chosen
  - To realize some sort of "order" or "broken symmetry", (for example, magnetic order)...there could be more than one order present (for example, superconductivity and magnetism)
  - To enforce some sort of "correlation" that we "simply" know exists

  and can include all of the "effects" above
- ...your guess is *not* as *good* as mine!

Variational Principle vs. MFT

- Mean Field theory
  - Replace H by H_{MF} which is usually quadratic
  - Use the Feynman identity $F \leq F_{MF} + \langle H - H_{MF} \rangle_{MF}$ (F is free energy)
  - Kills "fluctuations"
- Variational Principle
  - Works with the *full* Hamiltonian
  - Non-perturbative
  - *Well designed* wavefunctions can include fluctuations above MFT
- Usually MFT provides us with intuitive starting point...we can then "well design" the variational wavefunction to include the fluctuations that we miss

Overall Strategy of Variational Approach

Summary of Variational Approach

1. Design a ground state $|\Psi(\alpha_i)\rangle$
2. Energy function

$$E(\alpha_i) = \frac{\langle \Psi(\alpha_i)|H|\Psi(\alpha_i)\rangle}{\langle \Psi(\alpha_i)|\Psi(\alpha_i)\rangle}$$

3. Find α_i^m that minimize (extremize) $E(\alpha_i)$ and obtain $|\Psi_G\rangle$
4. Study $|\Psi_G\rangle$

- This explains the "Variational" part of VMC
- ...
- But...why Monte Carlo?

Variational Approach: The Difficulty

- In many cases the variational programme can be carried out analytically where we have a well controlled analytical expression for the state, e. g., BCS state
- In most problems of interest we *do not have a simple enough* analytical expression for the wavefunction (e. g., Gutzwiller wavefunction $|\Psi_{gutz}\rangle = g^D|\Psi_{free}\rangle$)
- In many of these cases we have expressions for the wavefunction which "look simple in real space", say, $\Psi_\alpha(r_{1\uparrow}, r_{2\uparrow}, \ldots, r_{N,\downarrow}, r_{1\downarrow}, r_{2\downarrow}, \ldots, r_{N,\downarrow})$, where $r_{i\sigma}$ are the coordinates of our electrons on a lattice (we will work exclusively with lattices, most ideas can be taken to continuum in a straightforward way); Ψ_α has necessary permutation symmetries, and α subscripts reminds us of the underlying parameters
- Call $C \equiv (r_{1\uparrow}, r_{2\uparrow}, \ldots, r_{N,\downarrow}, r_{1\downarrow}, r_{2\downarrow}, \ldots, r_{N,\downarrow})$ a *configuration* of the electrons

Variational Approach: The Difficulty

- Now,

$$E(\alpha_i) = \frac{\sum_C \Psi^*_\alpha(C) H \Psi_\alpha(C)}{\sum_C \Psi^*_\alpha(C) \Psi_\alpha(C)}$$

  i.e., we need to do a sum over *all* configurations C of the our $2N$ electron system
- Note that in most practical cases we need sum the denominator as well, since we use *unnormalized* wavefunctions!
- Sums...how difficult can they be?
- Consider 50 $\uparrow$ electrons, and 50 $\downarrow$ electrons on a lattice with 100 sites....How many configurations are there?

$$\text{Num. Configurations} \sim 10^{60}\text{!!!!}$$

- And this *is* the difficulty!
- ...
- Solution...use Monte Carlo method to perform the sum!

"Monte Carlo" of VMC

- How do we use Monte Carlo to evaluate $E(\alpha_i)$?
- Use the following trick Poor Notation Warning: $H\Psi(C) \equiv \langle C|H|\Psi\rangle$

$$\begin{aligned} E(\alpha_i) &= \frac{\sum_C \Psi^*_\alpha(C) H\Psi_\alpha(C)}{\sum_C \Psi^*_\alpha(C)\Psi_\alpha(C)} = \frac{\sum_C \Psi^*_\alpha(C)\Psi_\alpha(C)\ \frac{H\Psi_\alpha(C)}{\Psi_\alpha(C)}}{\sum_C \Psi^*_\alpha(C)\Psi_\alpha(C)} \\ &= \sum_C P(C)\frac{H\Psi_\alpha(C)}{\Psi_\alpha(C)} \end{aligned}$$

where

$$P(C) = \frac{|\Psi_\alpha(C)|^2}{\sum_C \Psi^*_\alpha(C)\Psi_\alpha(C)}$$

is the probability of the configuration C; obviously $\sum_C P(C) = 1$

- Note that we *do not know* the denominator of $P(C)$
- For any operator O

$$\langle O\rangle = \sum_C P(C)\frac{O\Psi_\alpha(C)}{\Psi_\alpha(C)}$$

Idea of Monte Carlo Sums

- Key idea is *not* to sum over all configurations C, but to visit the "most important" configurations and add up their contribution
- The most important configurations are those that have "high" probability..., but we *do not know* the denominator of $P(C)$
- Need to develop a scheme where we start with a configuration C_1 and "step" to another configuration C_2 comparing $P(C_1)$ and $P(C_2)$...and continue on
- Thus we do a "walk" in the space of configurations depending on $P(C)$...spending "most of our time" in high probability configurations...this is *importance sampling*
- Goal: construct a set of rules (algorithm) to "step" in the configuration space that performs the necessary importance sampling
- Such a stepping produces a sequence configurations a function of steps or "time"...but how do we create this "dynamics"?

Markov Chains

- Let us set notation: Label all the configurations (yes, all 10^{60}) using natural numbers $C_1, C_2 \ldots C_m \ldots$ etc; we will use $P(1) \equiv P(C_1)$, and in general $P(m) \equiv P(C_m)$ and $\sum_C \equiv \sum_m$
- We construct transition (Markov) matrix $W(n, m) \equiv W(n \leftarrow m)$ which defines the probability of moving from the configuration m to configuration n in a step, we consider only Ws that are independent of time
- The probability of taking a step from $m \rightarrow n$ is independent of how the system got to the state m...such stochastic processes are called as Markov chain
- Clearly $\sum_n W(n, m) = 1$, and $W(n, m) \geq 0$ Exercise: If λ is a right eigenvalue of the matrix $\mathbb{W}$, show that $|\lambda| \leq 1$.

Master Equation

- Question: Given a Markov matrix $\mathbb{W}$, and the knowledge that the probability distribution over the configuration space at step t is $\mathbb{P}(t)$ ($\mathbb{P}$ is the column $P(m)$), what is $\mathbb{P}(t+1)$?
- Clearly

$$P(n,t+1) = \sum_m W(n,m)P(m,t) \quad \mathbb{P}(t+1) = \mathbb{W}\mathbb{P}(t)$$

- How does the probability of a state change with time?

$$P(n,t+1) - P(n,t) = \sum_m W(n,m)P(m,t) - \sum_m W(m,n)P(n,t)$$

...the *Master equation*

- For a "steady" probability distribution

$$\begin{aligned} \sum_m W(n,m)P(m) - \sum_m W(m,n)P(n) &= 0 \\ \implies \sum_m W(n,m)P(m) &= P(n) \implies \mathbb{W}\mathbb{P} = \mathbb{P} \end{aligned}$$

...i.e., $\mathbb{P}$ is a right eigenvector of the Markov matrix $\mathbb{W}$ with unit eigenvalue!

Markov Chains...a bit more

- For our purpose, need to construct a Markov matrix $\mathbb{W}$ for which our $\mathbb{P}$ is an eigenvector...how do we do this?
- We define the *visit probability* $V(n, m; t)$ is the probability that the system reaches state n at time t for the first time given that the system was in configuration m at time 0 Exercise: Express $\mathbb{V}(t)$ in terms of $\mathbb{W}$
- The quantity $V(n, m) = \sum_t V(n, m; t)$ is the *total visit probability* of n from m
- If $V(n, m) \neq 0, \forall n, m$, i. e., any state can be reached from any other state, then Markov chain is said to be *irreducible*

Markov Chains...a bit more

- A state m is called *recurrent* if $V(m,m) = 1$, i.e., and the mean recurrence time is $t_m = \sum_t tV(m,m;t)$; if $t_m < \infty$, the state is called *positive recurrent*; if all states are positive recurrent, the chain is called *ergodic*
- A chain is *aperiodic* if no state repeats in a periodic manner
- *Fundamental theorem of Irreducible Markov Chains:* An ergodic aperiodic irreducible Markov chain has a unique stationary probability distribution
- We now need to construct an irreducible chain, i. e., the *key* point is that every state must be reachable from every other state
- The other conditions (positive recurrence) is easier to satisfy since our configuration space is finite albeit large

Detailed Balance

- How do we choose an irreducible chain whose stationary distribution is *our* distribution? Clearly, there is no unique choice!
- We can choose $\mathbb{W}$ in such a way that

$$W(n,m)P(m) = W(m,n)P(n)$$

  and this will clearly mean that $\mathbb{P}$ is the right eigenvector of $\mathbb{W}$...this condition is called the *detailed balance* condition
- Now, we are ready to construct an appropriate $\mathbb{W}$, define

$$W(n,m) = A(n,m)S(n,m)$$

  where $S(n,m)$ is called the "suggestion probability" i.e., the probability of suggesting a state n to move to, when we are at m, and $A(n,m)$ is called the "acceptance probability"
- Let us suppose that we have "designed" a suggestion probability matrix...what is the acceptance probability matrix?

Acceptance Matrix

- We can use detailed balance and immediately the following equation for the acceptance matrix

$$\frac{A(n,m)}{A(m,n)} = \frac{S(m,n)P(n)}{S(n,m)P(m)} = \frac{S(m,n)|\Psi(n)|^2}{S(n,m)|\Psi(m)|^2} \equiv h(n,m)$$

  note that denominators are gone!
- We now posit $A(n,m)$ to be function of $h(n,m)$, i.e.,

$$A(n,m) = F(h(n,m))$$

- The first condition can be satisfied if the function F satisfies

$$F(y) = yF(1/y)$$

- We have lots of freedom...we can choose *any* function that satisfies the above condition!

Acceptance Matrix: Popular Choices

- Metropolis

$$F(y) = \min\{1, y\} \implies A(n,m) = \min\left\{1, \frac{S(m,n)|\Psi(n)|^2}{S(n,m)|\Psi(m)|^2}\right\}$$

- Heat Bath

$$F(y) = \frac{y}{1+y} \implies A(n,m) = \frac{S(m,n)|\Psi(n)|^2}{S(m,n)|\Psi(n)|^2 + S(n,m)|\Psi(m)|^2}$$

Suggestion Matrix

- Simplest suggestion matrix: Based on single electron moves
- Single electron moves: Successive configurations differ only in the position of a *single electron*
  - At any step pick an electron at random
  - Move the electron from its current position to a new position also picked at random
  - We have

$$S(n,m) = \frac{1}{N_{electrons} \times (N_{sites} - 1)}$$

  Note that $S(m,n) = S(n,m)$
- Metropolis acceptance matrix becomes

$$\min\left\{1, \frac{|\Psi(n)|^2}{|\Psi(m)|^2}\right\}$$

...we have constructed our Markov matrix $\mathbb{W}$ Question: Does our $\mathbb{W}$ produces an irreducible chain?

..and some Final Touches

- We now generate a sequence of configurations m_k starting from some random initial configuration using our Markov matrix $\mathbb{W}$...say we take N_{MC} steps
- The key result of importance sampling

$$E(\alpha_i) = \frac{1}{N_{MC}} \sum_{k=1}^{N_{MC}} \frac{H\Psi_\alpha(m_k)}{\Psi_\alpha(m_k)}$$

...and this work for other operators as well

$$\langle O \rangle_\alpha = \frac{1}{N_{MC}} \sum_{k=1}^{N_{MC}} \frac{O\Psi_\alpha(m_k)}{\Psi_\alpha(m_k)}$$

Variational Monte Carlo

VMC Summary

1. Start with a random configuration
2. For $k = 0, N_{MC}$
   - In configuration m_k, pick an electron at random, suggest a random *new* position for this electron, call this configuration m'_k
   - Accept m'_k as m_{k+1} with probability $\min\left\{1, \frac{|\Psi(m'_k)|^2}{|\Psi(m_k)|^2}\right\}$, if m'_k is not accepted, set $m_{k+1} = m_k$
   - Accumulate $\frac{O\Psi_\alpha(m_{k+1})}{\Psi_\alpha(m_{k+1})}$
3. Calculate necessary averages for $E(\alpha_i)$
4. Optimize over α_i, obtain $|\Psi_G\rangle$
5. Study $|\Psi_G\rangle$

Comments on VMC

- Note that our starting configuration in most practical situations is sampled from a *different* probability distribution from the one we are interested in!
- If we take sufficiently large number of steps we are *guaranteed* by the fundamental theorem that we will "reach" our desired distribution
- How fast we attain our desired distribution depends next largest eigenvalue of $\mathbb{W}$...it might therefore be desirable to design $\mathbb{W}$ such that all other eigenvalues of $\mathbb{W}$ are much less than unity
- Passing remark: In VMC we know which $\mathbb{P}$ we want and we *construct* a $\mathbb{W}$ to sample $\mathbb{P}$...In "Green's Function Monte Carlo" (GFMC) we *have* a $\mathbb{W} = e^{-H}$, we start with some $\mathbb{P}(\equiv |\Psi\rangle)$ and *project out* the ground state $\mathbb{P}_{GroundState}(\equiv |\Psi_G\rangle)$ by repeated application of $\mathbb{W}$

VMC Computational Hardness

- How hard is VMC?
- For every step, once we make a suggestion for a new configuration, we need to evaluate the ratio $\frac{|\Psi(m_k')|^2}{|\Psi(m_k)|^2}$
- Now Ψ is usually obtained in a determinental form. If there are $2N$ electrons, we usually have determinants of order $N \times N$
- How hard is the calculation of a determinant? This is an N^3 process...
- Not too good, particularly since we have to optimize with respect to α_i...we like things to be $O(N)$ hard!
- ...
- ...all is *not* lost!

Faster VMC

- Note that throughout our calculation, we need only the ratio of determinants, not the determinants themselves
- To illustrate the idea behind this, consider spinless fermions; we have a configuration m given by a wavefunction $|\Psi\rangle$ and a configuration n given by a wavefunction $|\Phi\rangle$ which differ by the *position of a single electron* I, r_I *and* r'_I; written in terms of matrices

$$[\Psi] = \begin{pmatrix} \psi_{a_1}(r_1) & \cdots & \psi_{a_1}(r_I) & \cdots & \psi_{a_1}(r_N) \\ \vdots & \cdots & \vdots & \vdots & \\ \psi_{a_N}(r_1) & \cdots & \psi_{a_N}(r_I) & \cdots & \psi_{a_N}(r_N) \end{pmatrix}$$

and

$$[\Phi] = \begin{pmatrix} \psi_{a_1}(r_1) & \cdots & \psi_{a_1}(r'_I) & \cdots & \psi_{a_1}(r_N) \\ \vdots & \cdots & \vdots & \vdots & \\ \psi_{a_N}(r_1) & \cdots & \psi_{a_N}(r'_I) & \cdots & \psi_{a_N}(r_N) \end{pmatrix}$$

where ψ_{a_i} are some one particle states (which usually depend on α_i)

Faster VMC

- We need $\frac{\det[\Phi]}{\det[\Psi]}$...key point:[$\Phi$] and [$\Psi$] differ only in one column!
- Now

$$\begin{aligned}
\sum_k \Phi^{-1}_{ik}\Phi_{kj} = \delta_{ij} \implies \sum_k \mathrm{Cof}\Phi_{ki}\Phi_{kj} &= \det[\Phi]\delta_{ij} \\
\implies \sum_k \mathrm{Cof}\Phi_{kl}\Phi_{kl} &= \det[\Phi] \\
\mathrm{Cof}\Phi_{kl} = \mathrm{Cof}\Psi_{kl} \implies \det[\Phi] &= \sum_k \mathrm{Cof}\Psi_{kl}\Phi_{kl} \\
\implies \frac{\det[\Phi]}{\det[\Psi]} &= \sum_k \Psi^{-1}_{kl}\Phi_{kl}
\end{aligned}$$

  which is certainly $O(N)$

- Note that we need to know Ψ^{-1}, and thus have to *store* it at every step!
- When we accept a suggested configuration, we will have to recalculate Ψ^{-1} which, again, appears to be $O(N^3)$!

Fast Update of Ψ^{-1} (Sherman-Morrison-Woodbury)

- On acceptance of the suggested configuration, we need to compute Φ^{-1} which will be the new Ψ^{-1} for the next step
- Calling $r = \frac{\det[\Phi]}{\det[\Psi]}$, we immediately have

$$\Phi^{-1}_{lj} = \frac{1}{r}\Psi^{-1}_{lj}$$

- Other rows of Φ^{-1} can be obtained as

$$\Phi^{-1}_{ij}\Big|_{i\neq l} = \Psi^{-1}_{ij} - \beta_i \Psi^{-1}_{lj}, \quad \beta_i = \frac{1}{r}\sum_k \Psi^{-1}_{ik}\Phi_{kl}$$

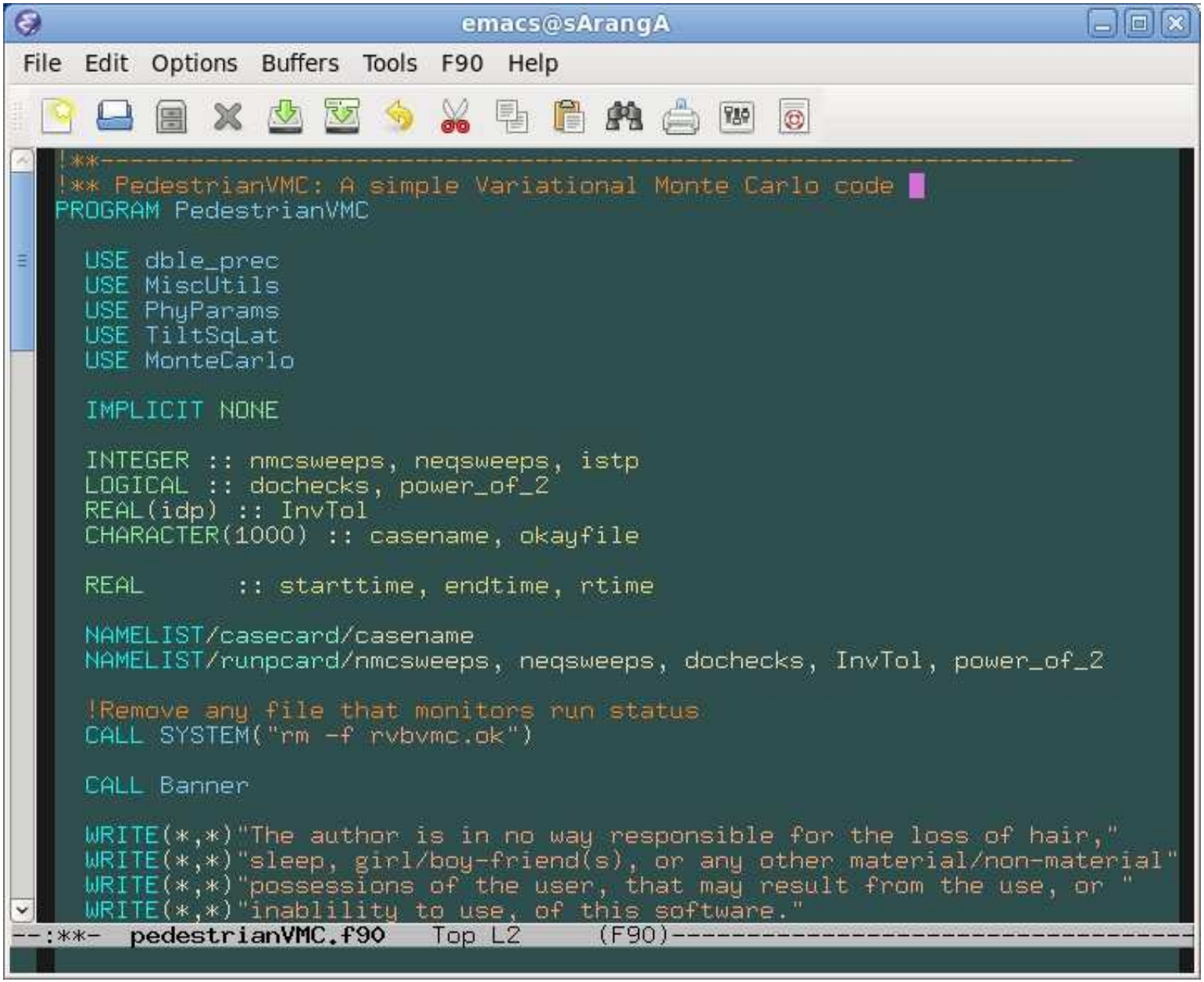
  which is certainly an $O(N^2)$ process
- Note that care has to be exercised in using this procedure to update Ψ^{-1} due to accumulation of (round-off) errors...every so often we must generate Ψ^{-1} from the positions of the electrons using an $O(N^3)$ algorithm
- In short VMC, at its best, is $O(N^2)$ hard! Note that calculation of correlation functions can be harder

Variational Monte Carlo

VMC Summary

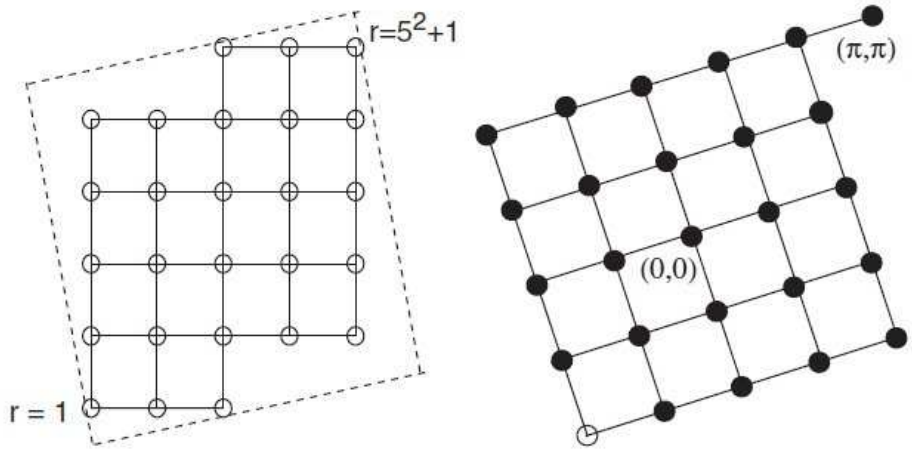
1. Start with a random configuration
2. For $k = 0, N_{MC}$
   - In configuration m_k, pick an electron at random, suggest a random *new* position for this electron, call this configuration m'_k
   - Accept m'_k as m_{k+1} with probability $\min\left\{1, \frac{|\Psi(m'_k)|^2}{|\Psi(m_k)|^2}\right\}$, if m'_k is not accepted, set $m_{k+1} = m_k$
   - Update Ψ^{-1} if $m_{k+1} = m'_k$ using SMH formula (check every so often and perform a full update)
   - Accumulate $\frac{O\Psi_\alpha(m_{k+1})}{\Psi_\alpha(m_{k+1})}$
3. Calculate necessary averages for $E(\alpha_i)$
4. Optimize over α_i, obtain $|\Psi_G\rangle$
5. Study $|\Psi_G\rangle$

Free VMC Code pedestrianVMC



pedestrianVMC Examples

- We will work on the square lattice, using a tilted configuration, number of sites go as L^2+1 (L has to be odd)



(Paramekanti, Randeria and Trivedi, *PRB* (2004))

- Hubbard model

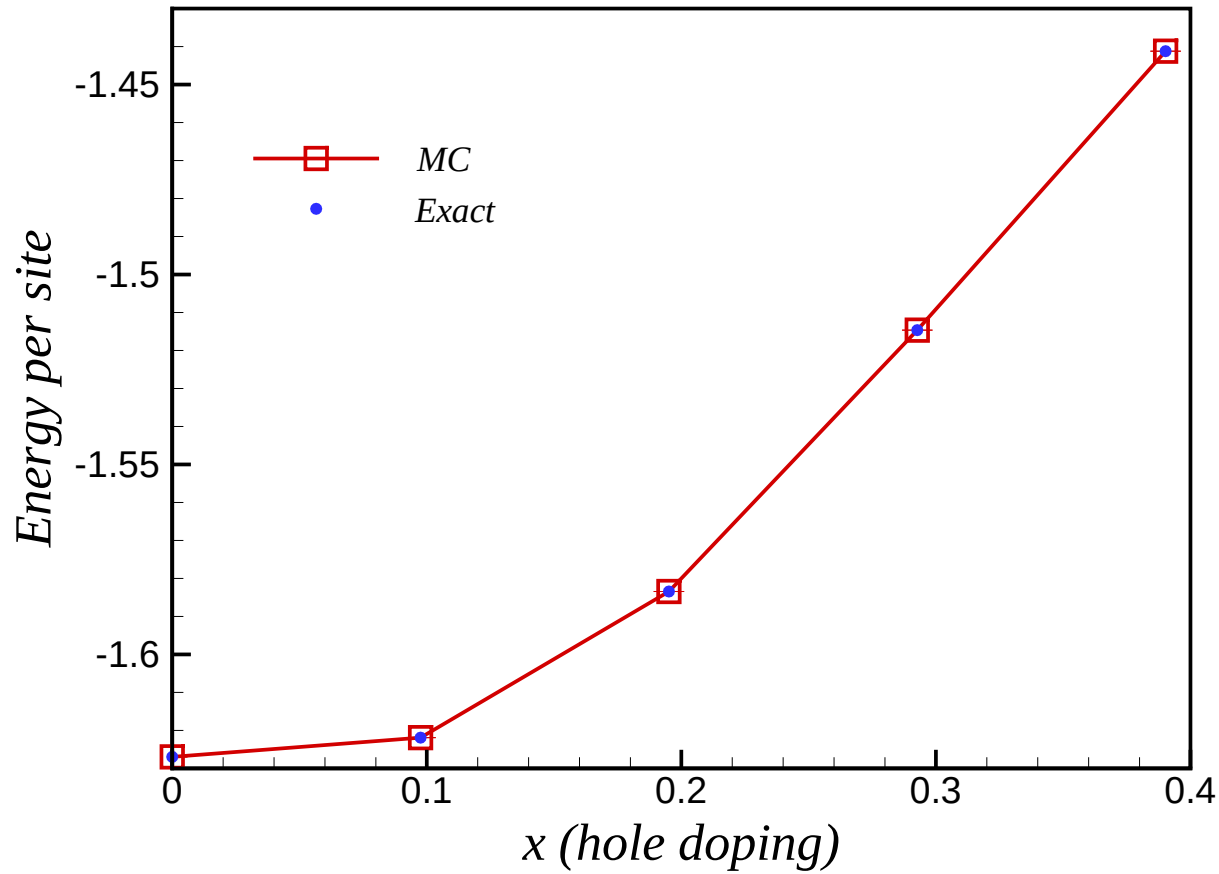
$$-\sum_{\langle ij\rangle} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

we will consider two cases: $U = 0$ (free electrons) and $U = \infty$

- Number of electrons in the lattice is characterized by x the doping from the *half filled* state (one electron for each lattice site

Free Gas ($U = 0$)

- Guess for the ground state $|\Psi\rangle = |FS\rangle$
- Suggestion matrix using single electon moves

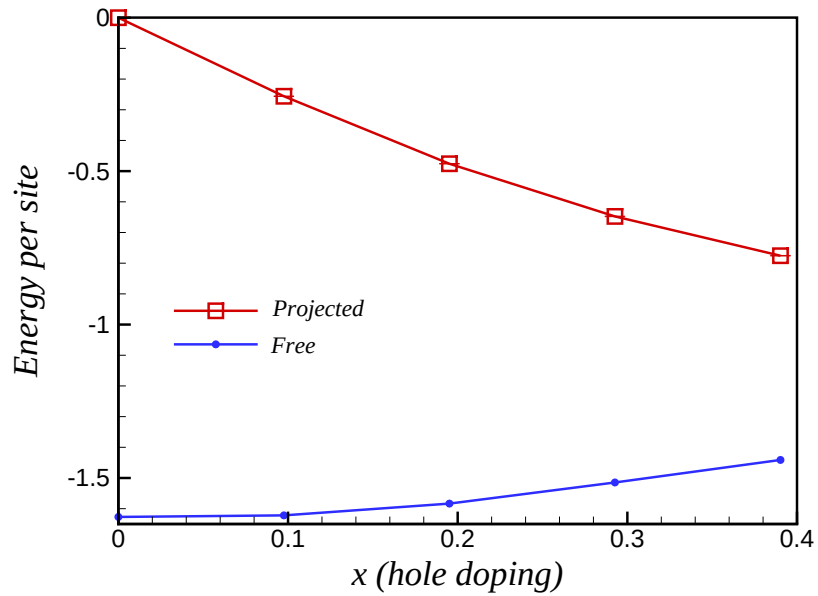


$L = 9, N_{MC} = 4000$

- ...note we have sampled only 10^{-55} of the possible configurations!

Extremely Correlated Liquid ($U = \infty$)

- Guess $|\Psi\rangle = P|FS\rangle$ – Projected Fermi Liquid...In terms of real space wavefunctions the P means this: $\forall$ configurations C with at least one doubly occupied site the wave function $\Psi(C)$ vanishes...double occupancy is *strictly forbidden*
- Suggestion matrix using single electon moves ...does NOT work! Need to introduce *spin flip* moves ... this is actually a two-electron move



$L = 9, N_{MC} = 16000$

How well are we doing?

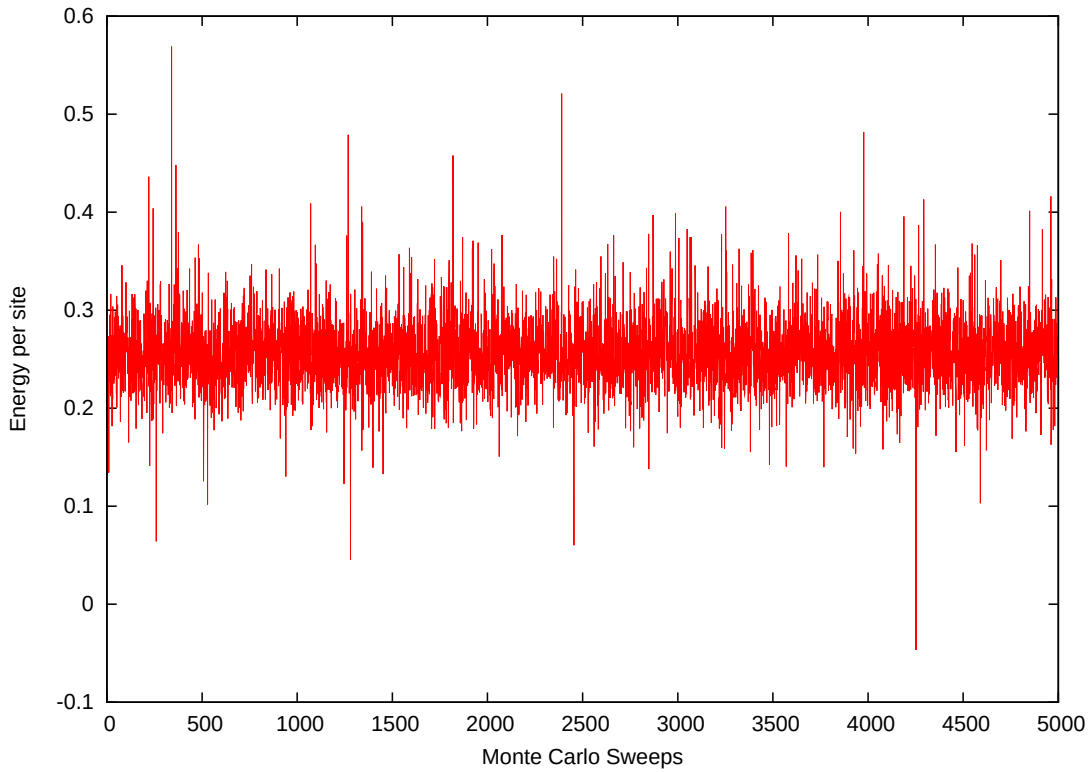
- Sampling Error
- Systematic Error (Random number generator etc.)
- Finite Size Effects
- ...
- Bugs

How well are we doing?

- We use the estimator

$$\langle O \rangle = \frac{1}{N_{MC}} \sum_k O_k, \qquad O_k \equiv \frac{O\Psi(m_k)}{\Psi(m_k)}$$

for the expectation value of the operator



- We are sampling a *finite chain*... leads to *sampling error*

Sampling Error

- Suppose we have a Gaussian distribution, want to find its mean value by sampling...if we perform N *independent* samplings, we can estimate the mean with a standard error of $\sigma/\sqrt{N}$ where σ is the variance of the Gaussian
- In our case we can estimate the error as

$$\begin{aligned}
\varepsilon_O^2 &= \left\langle \left(\frac{1}{N_{MC}} \sum_k O_k \right)^2 \right\rangle - \left\langle \frac{1}{N_{MC}} \sum_k O_k \right\rangle^2 \\
&= \frac{1}{N_{MC}^2} \sum_{jk} \langle (O_j - \langle O \rangle)(O_k - \langle O \rangle) \rangle \\
&= \frac{1}{N_{MC}} \left(\sum_k \langle (O_k - \langle O \rangle)^2 \rangle \right) + \frac{1}{N_{MC}^2} \sum_{j \neq k} \langle (O_j - \langle O \rangle)(O_k - \langle O \rangle) \rangle \\
&= \frac{1}{N_{MC}} (\sigma^O)^2 + \frac{1}{N_{MC}} \sum_{k=1}^{N_{MC}} (1 - \frac{k}{N_{MC}}) \lambda_k^O
\end{aligned}$$

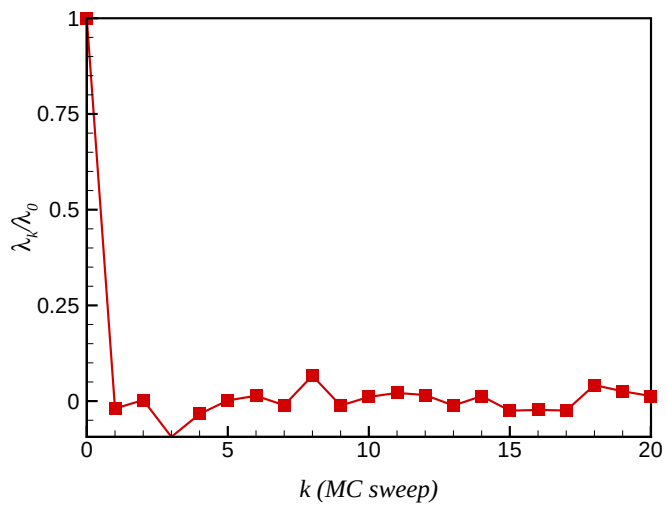
Sampling Error

- Autocorrelation function

$$\lambda_k^O = \langle (O_k - \langle O \rangle)(O_0 - \langle O \rangle) \rangle$$

clearly, $\sigma^O = \sqrt{\lambda_0^O}$

- We see in addition to the variance, the auto correlation function also contributes to the errors
- *Always* look at auto-correlation functions



$U = \infty, x = 0.1, L = 9$

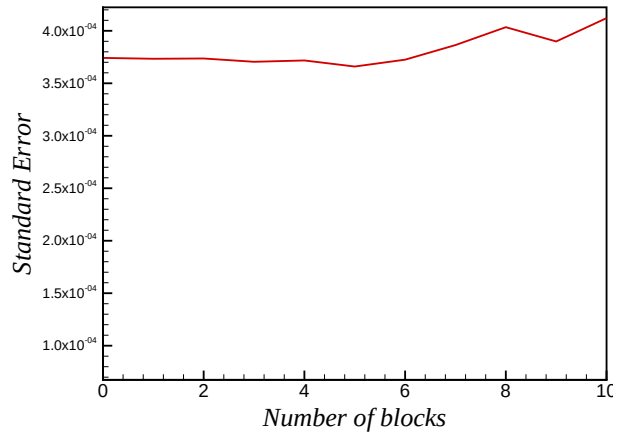
Not bad!

Sampling Error: Blocking

- There is a nice trick to calculate the error of auto-correlated data *without calculating autocorrelations*...this is called blocking...attributed to Wilson
- The idea is same as Kadanoff' block spin RG trick... Start with the data of size N_{MC} which for convenience we can take to be a power of 2, calculate its standard error ε_0
- Now generate new data which is of size $N_{MC}/2$ by $O_k^{blocked} = (O_{2k} + O_{2k+1})/2$ and calculate its standard error ε_1...the subscript "1" stands for first level of blocking
- Continue this procedure (you need sufficient data) and plot ε_b as a function b where b is the number of block transformations applied
- Pick the plateau value for the error

Sampling Error: Blocking

- Our example, we are doing okay



$$U = \infty, x = 0.1, L = 9, N_{MC} = 2^{15}$$

- An example with strong auto-correlations

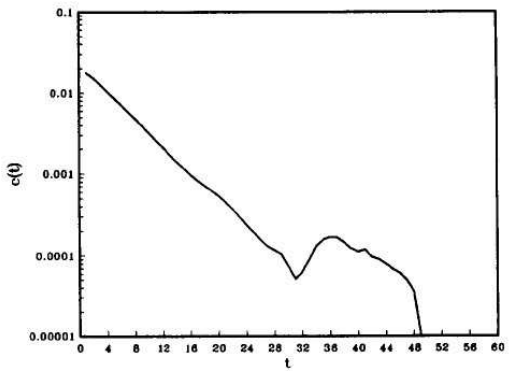


FIG. 1. c_t vs t. c_t was computed from $n = 2^{17}$ measurements of the magnetization $(x_t)_{t=1,\ldots,n}$ using the defining Eq. (8). For $0 \le t \le 16$ $c_t \simeq 0.022 \exp(-t/5.1)$.

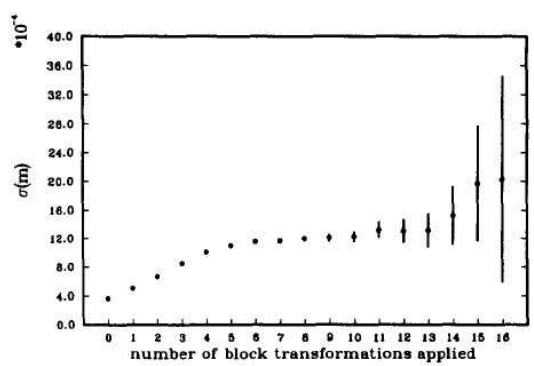
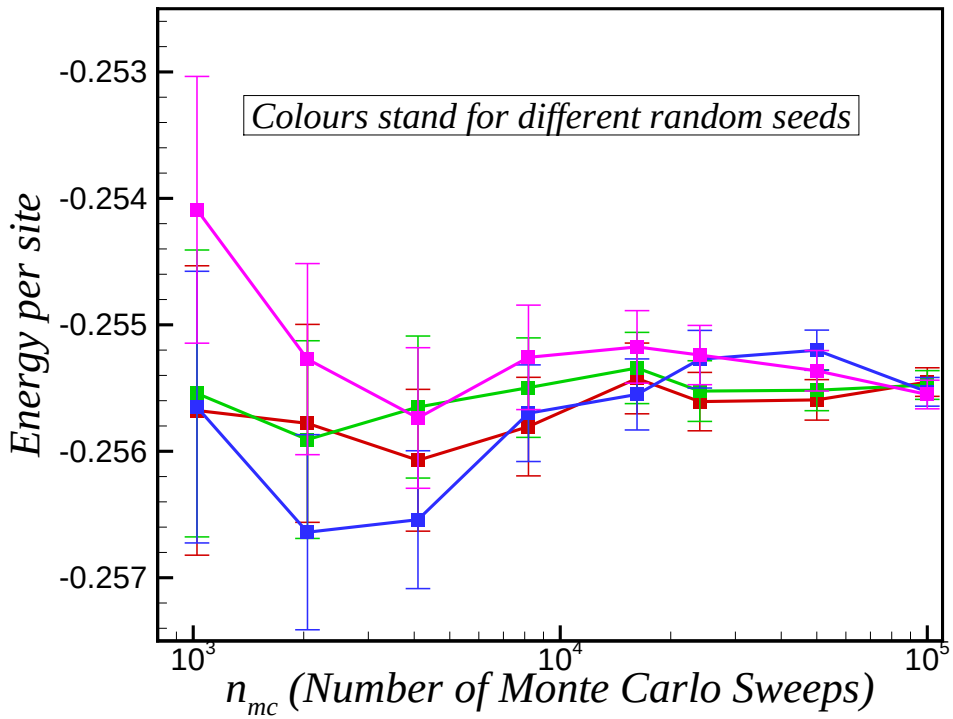


FIG. 3. Estimate for $\sigma(m)$ obtained with the blocking method. After ~ 6 block transformations the estimates remain constant within error bars at 0.0012.

(Flyvbjerg and Petersen, *JCP* (1984))

Equilibration

- How
  to check for equilibration...run calculations with different random seeds!

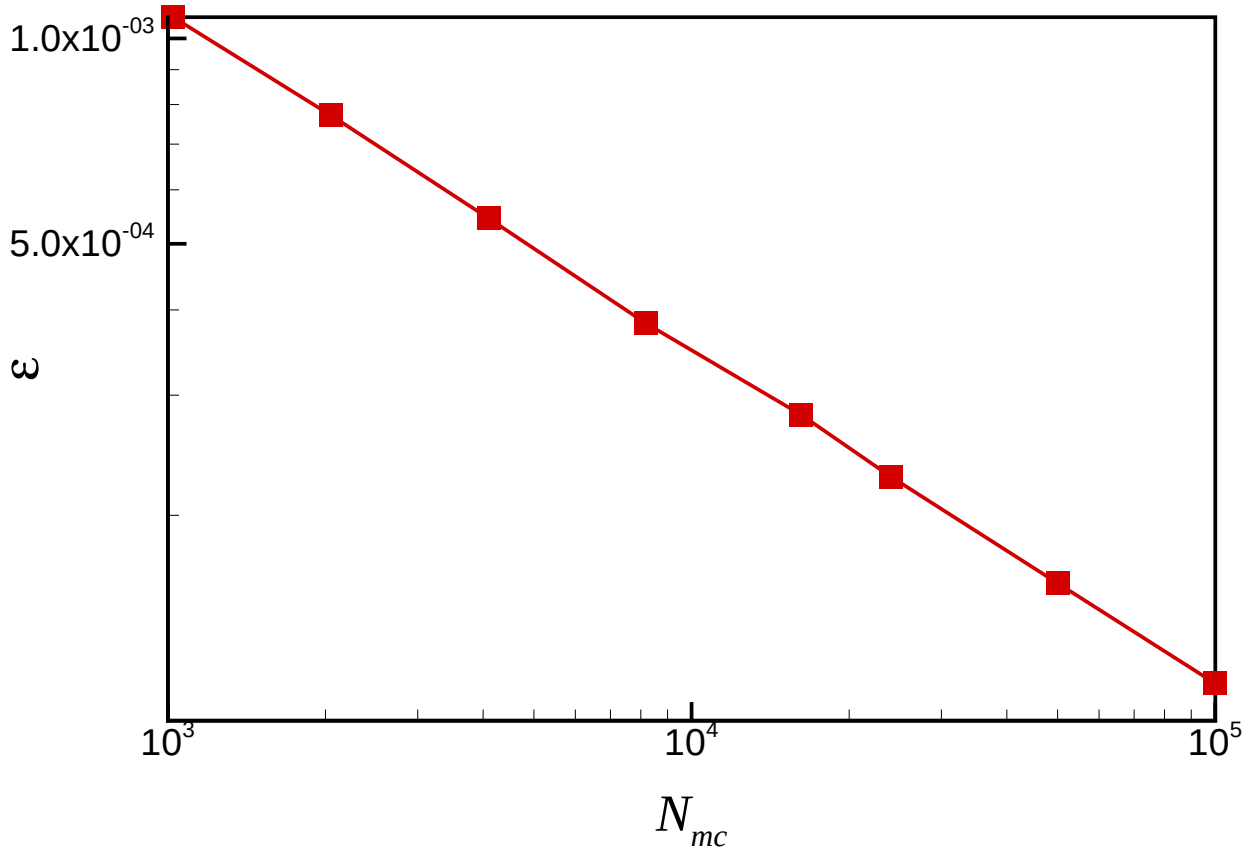


$U = \infty, x = 0.1, L = 9$

- "Large" seed-dependence is a sure sign of non-equilibration...we are doing okay when $N_{MC} \geq 10000$ in this example

One Final Check

- How well can we do?
  If everything is okay the error should fall of as $1/\sqrt{N_{MC}}$

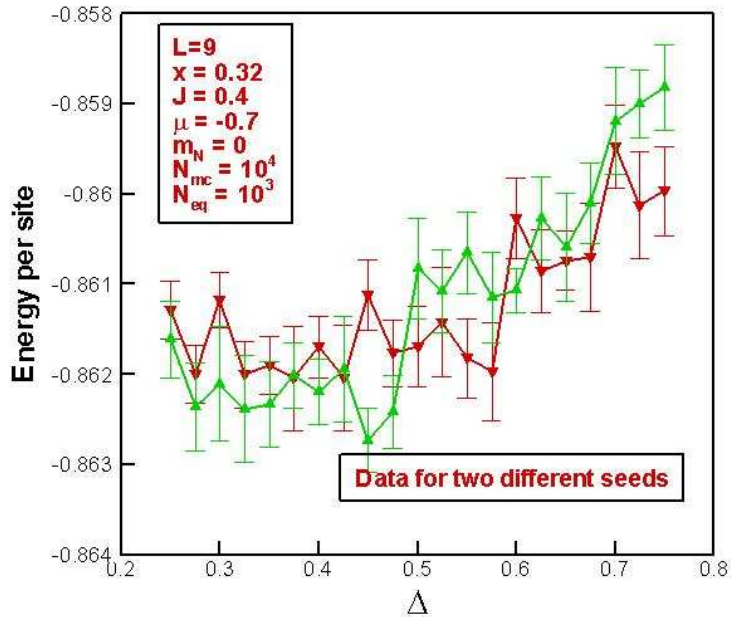


$U = \infty, x = 0.1, L = 9$

- We are doing pretty okay!...But, are we really?

Another Difficulty

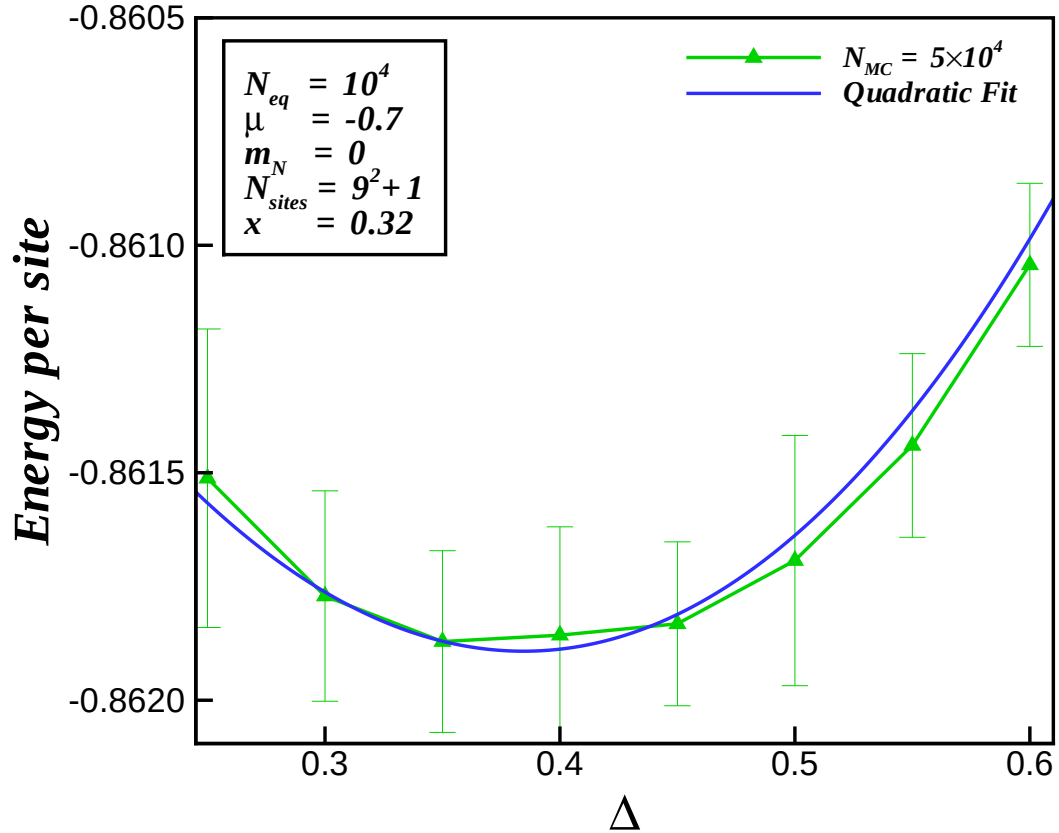
- When we want to optimize with respect to the variational parameters, we will have to evaluate the energy many times over...long that reduce error bars are prohibitive
- Shorter runs produce data that are bumpy, and seed dependent...



- The problem is particularly severe if the minimum is "shallow"...and becomes worse with increasing number of variational parameters

Difficulty Overcome: Parallelization

- "Seed parallelization" – Cloning



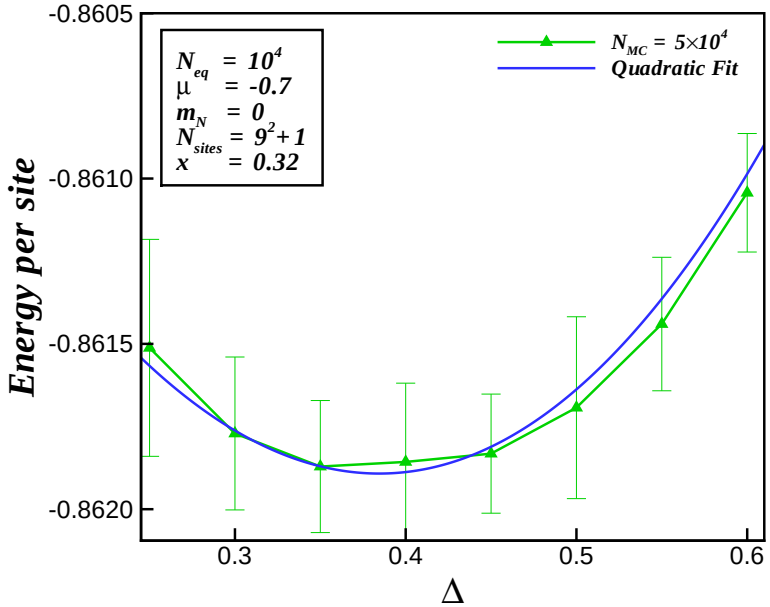
- Produces "smooth" enough data (we use up to 120 clones)

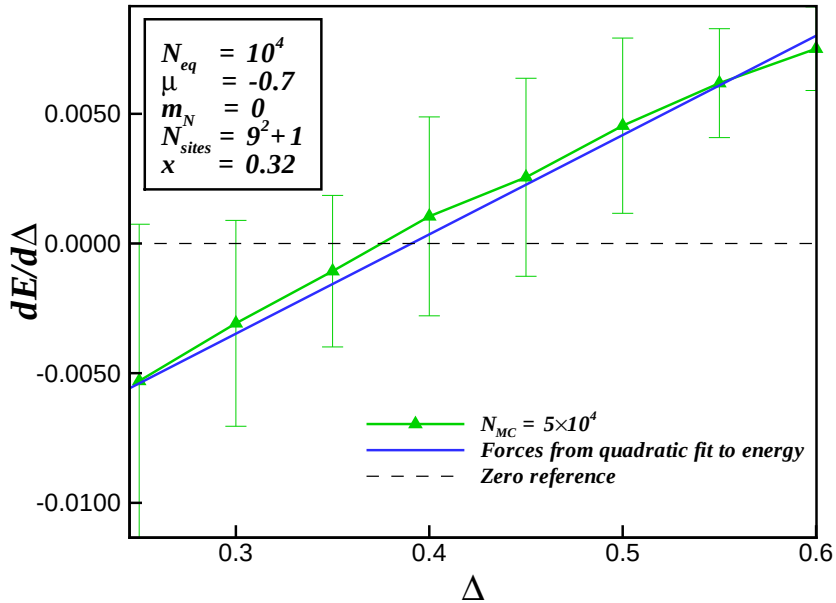
Optimizing Variational Parameters

- No derivative information
  - Direct search
  - Simplex method (use `amoeba` routine from Numerical Recipes)
  - Genetic algorithms?
- Method with derivative information

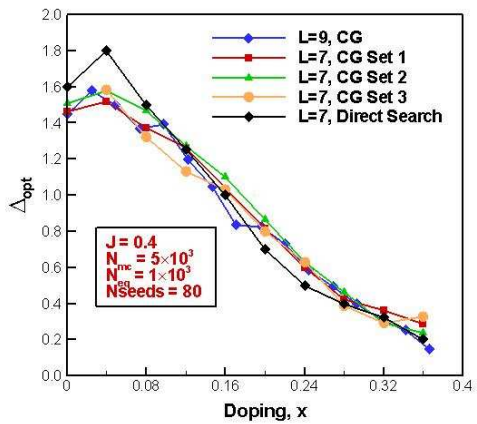
Results of Force Method

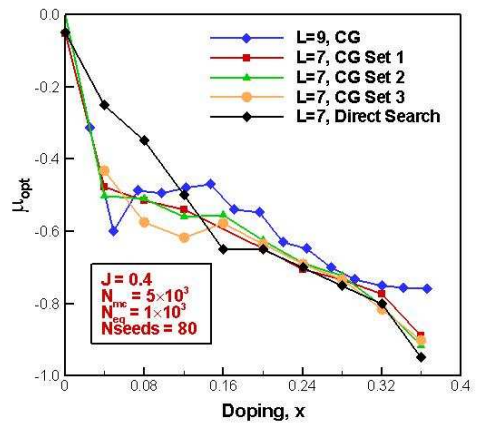
- Seed average forces





- Results for optimized variational parameters





Variational Monte Carlo

VMC Summary

1. Start with a random configuration
2. For $k = 0, N_{MC}$
   - In configuration m_k, pick an electron at random, suggest a random *new* position for this electron, call this configuration m'_k
   - Accept m'_k as m_{k+1} with probability min $\left\{1, \frac{|\Psi(m'_k)|^2}{|\Psi(m_k)|^2}\right\}$, if m'_k is not accepted, set $m_{k+1} = m_k$
   - Update Ψ^{-1} if $m_{k+1} = m'_k$ using SMH formula (check every so often and perform a full update)
   - Accumulate $\frac{O\Psi_\alpha(m_{k+1})}{\Psi_\alpha(m_{k+1})}$
3. Calculate necessary averages for $E(\alpha_i)$
4. Optimize over α_i, obtain $|\Psi_G\rangle$
5. Study $|\Psi_G\rangle$

- Finally, our answers will be only as good as our guess...

Applications to Superconductivity: Overview

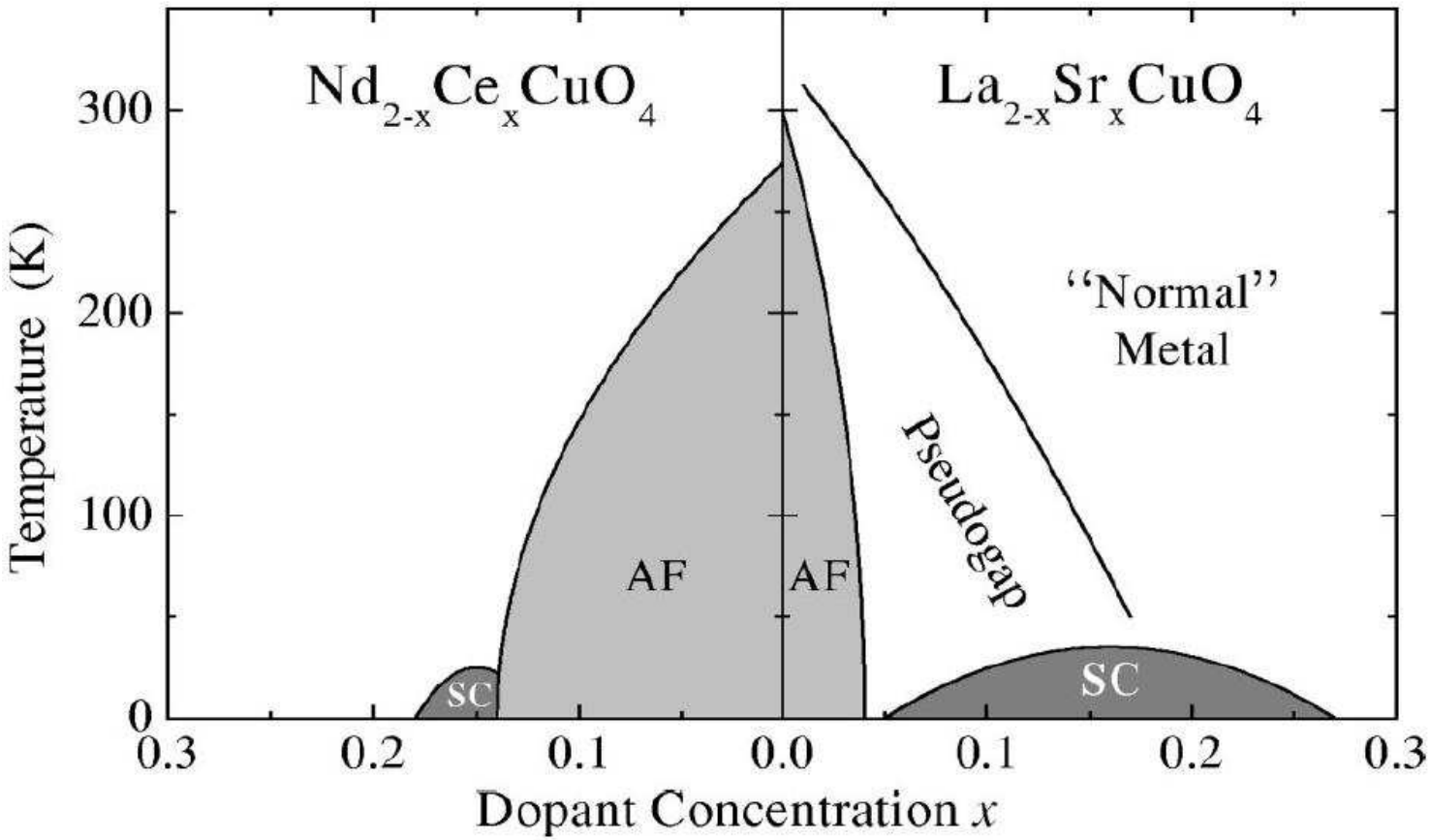
- Essential High T_c
- Models etc..
- RVB Wavefunction + VMC Results
- Material dependencies of the phase diagram
- Graphene

References on VMC in High T_c

- Gross et al., Giamarchi et al., Ogata et al., TKLee et al., PLee et al. and others
- Paramekanti, Randeria, Trivedi, *PRB* (2004) (see also, earlier *PRL*)
- (A2Z) Anderson, Lee, Randeria, Rice, Trivedi, Zhang, *JPCM* (2004)
- Recent comprehensive review: Edegger, Muthukumar, Gros *Adv. Phys* (2007)

Cuprate Phase Diagram

- Generic phase diagram

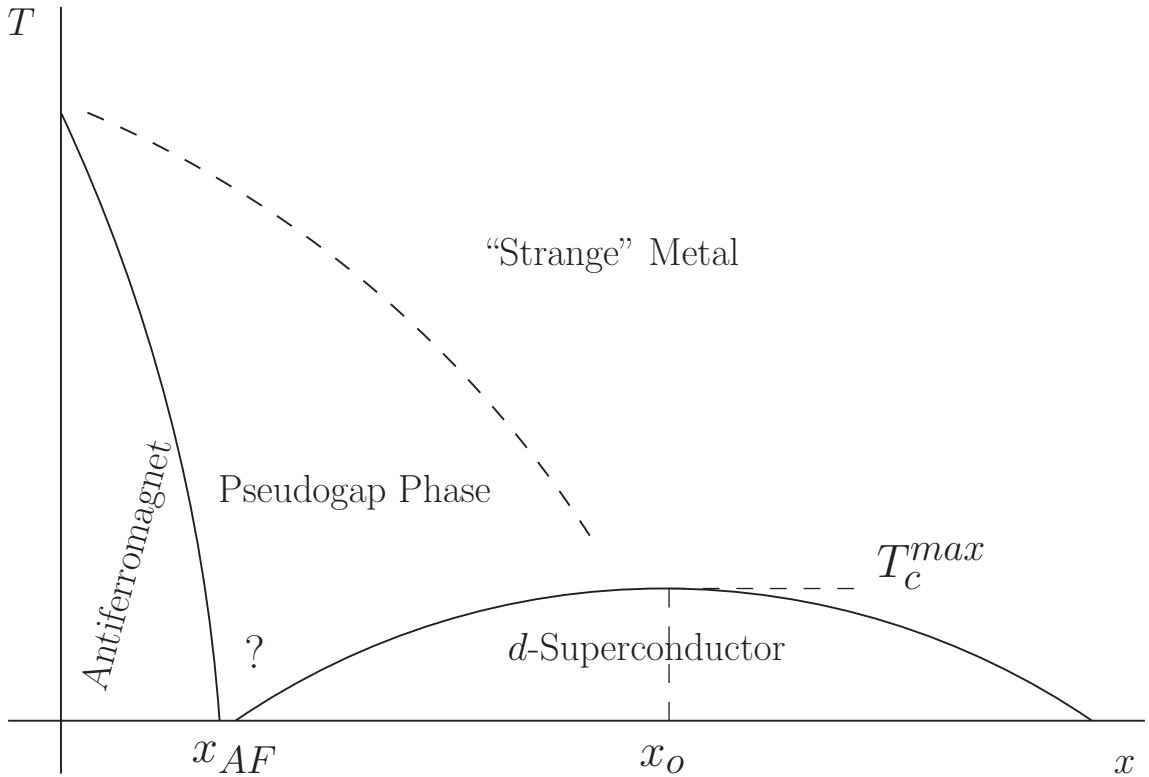


(Damascelli et al. 2003)

- Undoped system is a Mott insulator
- Note the electron-hole asymmetry

Cuprates: Phase Diagram

Key features



- x_{AF} – doping at which AF dies
- T_c^{max} – maximum superconducting T_c
- x_o – optimal doping

Model Hamiltonian

- What is the minimal model?
- One band model (Anderson et al.)
- Undoped system is a Mott insulator...must have large onsite repulsion
- Minimal model - one band Hubbard model

$$H_H = \underbrace{-\sum_{\langle ij \rangle} t_{ij}(c^\dagger_{i\sigma} c_{j\sigma} + h.c.) - \mu \sum_{i\sigma} n_{i\sigma}}_{K} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- Related tJ model

$$\begin{aligned} H_{tJ} &= P - \sum_{\langle ij \rangle} t_{ij}(c^\dagger_{i\sigma} c_{j\sigma} + h.c.)P - \mu \sum_{i\sigma} n_{i\sigma} \\ &\quad + \underbrace{J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right)}_{H_J} \end{aligned}$$

P stands for projection – hopping should not produce doublons

Are the two Models Related?

- Apply a canonical transformation on the Hubbard model to "project out" doubly occupied sector of the Hilbert space
- Canonical transformation $e^{iS}He^{-iS}$...this leads to

$$PH_HP = PKP + \underbrace{H_J + H_{K3site}}_{O(t^2/U)}$$

- J is now related to t and U as

$$J = \frac{4t^2}{U}$$

  can be understood from a two site model
- Typically $U \sim 10 - 12t$, $J/t \sim 0.3$, $t \sim 0.3 - 0.5eV$
- Note that $U \to \infty$ gives us

$$H_{U=\infty} = PKP$$

  which we had seen earlier

$U = \infty$ Revisited

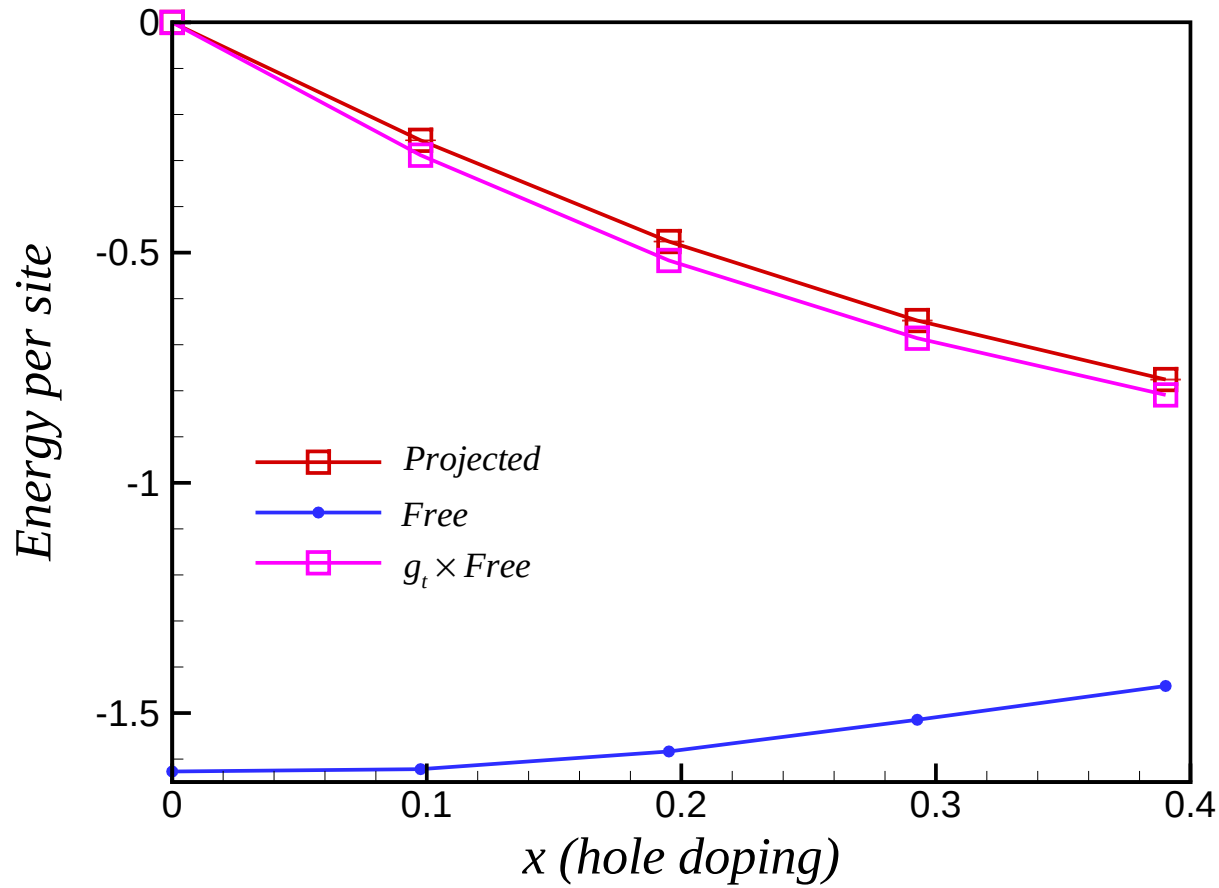
- Nothing can hop at half filling...what happens at a doping x?
- Ask the question: What is the relative probability an electron will find a hole on the neighbouring site?...this can be shown to be $g_t = \frac{2x}{1+x}$
- Suggests that

$$H = PKP \mapsto g_t K!$$

  which is now a "free particle" Hamiltonian!
- How well does this do?

$U = \infty$ Revisited

- Our guess for the ground state is $|\Psi\rangle = P|FS\rangle$...
- The "projected kinetic energy" is $\langle\Psi|H|\Psi\rangle = g_t\langle FS|K|FS\rangle$



$L = 9$

- Does okay?...looks like!

$U = \infty$ and the tJ model

- From the $U = \infty$ results, we see immediately that kinetic energy is badly "frustrated"
- What happens when we add the H_J to PKP?...this is the tJ model
- At zero doping ($x = 0$) we get

$$H_{tJ} \underbrace{=}_{x=0} J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

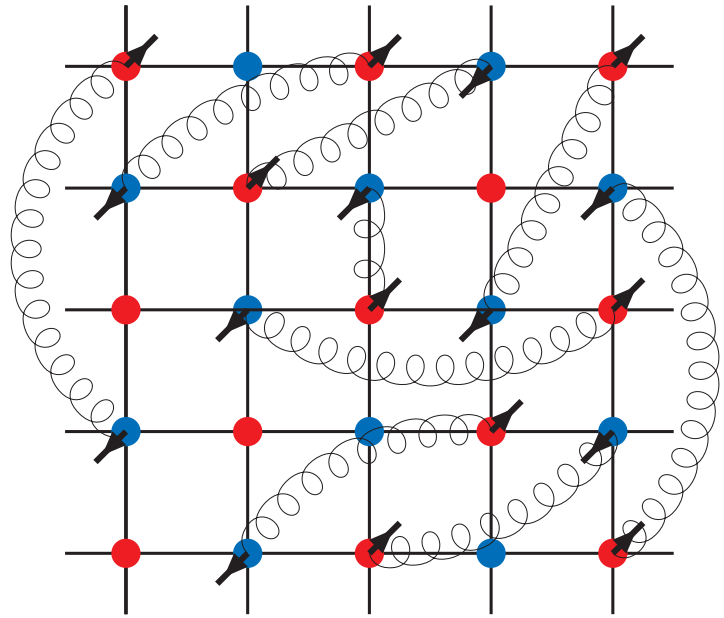
  which is the Heisenberg model...
- On a square lattice we know this has a Neél ground state (with a smaller staggered magnetization)

tJ model...effect of doping

- Projection badly frustrates kinetic energy...what is the effect of H_J on kinetic energy?
- H_j wants singlets...but this is "localizing" and frustrates the kinetic energy further...
- Expect
  - J to win over t at "small" doping...very little kinetic energy to be gained...lots of J energy to gained
  - At "large" doping expect kinetic energy to win
  - Doping where competition is most severe $2xt \sim J \Longrightarrow x \sim 0.15$!!
- Who wins?

Ground State at Finite Doping

- Actually, *both*, in a superconducting state!



- Both J and t can be satisfied by forming *resonating singlets* Idea embodied in the Resonating Valance Bond (RVB) state, Anderson (1987)
- How do we construct an RVB state?
- Will (can) it be a superconductor of the right pairing symmetry?

Mean Field Theory

- Keep projection aside...rewrite the tJ Hamiltonian as

$$H_{tJ} = K - J\sum_{ij} b_{ij}^{\dagger} b_{ij}$$

  where $b_{ij}^{\dagger} \sim (c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} - c_{i\downarrow}^{\dagger} c_{j\uparrow}^{\dagger})$
- Construct a meanfield Hamiltonian

$$H_{MF} = K - \sum_{ij} \Delta_{ij} b_{ij} + ...$$

  where $\Delta_{ij} \sim J\langle b_{ij}^{\dagger}\rangle ...$ is the "singlet pair amplitude"
- Translational invariance two pair amplitudes Δ_x and Δ_y — d symmetry is obtained by keeping $\Delta_x = \Delta$ and $\Delta_y = -\Delta$
- We now have a BCS like Hamiltonian, ground state

$$|dBCS\rangle = \prod_{k} (u_k + v_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger})|0\rangle$$

dRVB state

- The "guess" for the ground state is

$$|\Psi\rangle = P|dBCS\rangle = e^{\sum_k \phi_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}}|0\rangle \quad \phi_k = \frac{v_k}{u_k}$$

- For working on a lattice

$$\begin{aligned} |\Psi\rangle &= P\left(\sum_k \phi_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)^{N/2}|0\rangle \\ &= P\left(\sum_k \phi(i-j) c^\dagger_{i\uparrow} c^\dagger_{j\downarrow}\right)^{N/2}|0\rangle \end{aligned}$$

All our variational parameters are buried in $\phi(i-j)$, the "pair wavefunction"

Variational Wavefunction

- Given variational parameters construct ϕ
- Pick number of electrons N using doping $x = 1 - \frac{N}{N_L}$ (N_L number of sites)
- Variational wave function

$$P\Psi(\{r_{i\uparrow}, r_{j\downarrow}\}) = \begin{vmatrix} \phi(r_{1\uparrow} - r_{1\downarrow}) & \dots & \phi(r_{1\uparrow} - r_{N/2\downarrow}) \\ \vdots & \ddots & \vdots \\ \phi(r_{N/2\uparrow} - r_{1\downarrow}) & \dots & \phi(r_{N/2\uparrow} - r_{N/2\downarrow}) \end{vmatrix}$$

- Optimize, obtain the ground state, and study it

Superconducting order parameter

- The superconducting correlation function

$$F_{\alpha,\beta}(\mathbf{r}-\mathbf{r}') = \langle b^{\dagger}_{\mathbf{r}\alpha} b_{\mathbf{r}'\beta} \rangle$$

  $b^{\dagger}_{\mathbf{r}\alpha} = \frac{1}{2}(c^{\dagger}_{\mathbf{r}\uparrow} c^{\dagger}_{\mathbf{r}+\hat{\alpha}\downarrow} - c^{\dagger}_{\mathbf{r}\downarrow} c^{\dagger}_{\mathbf{r}+\hat{\alpha}\uparrow})$ creates a singlet on the bond $(\mathbf{r}, \mathbf{r}+\hat{\alpha})$, $\alpha = x, y$

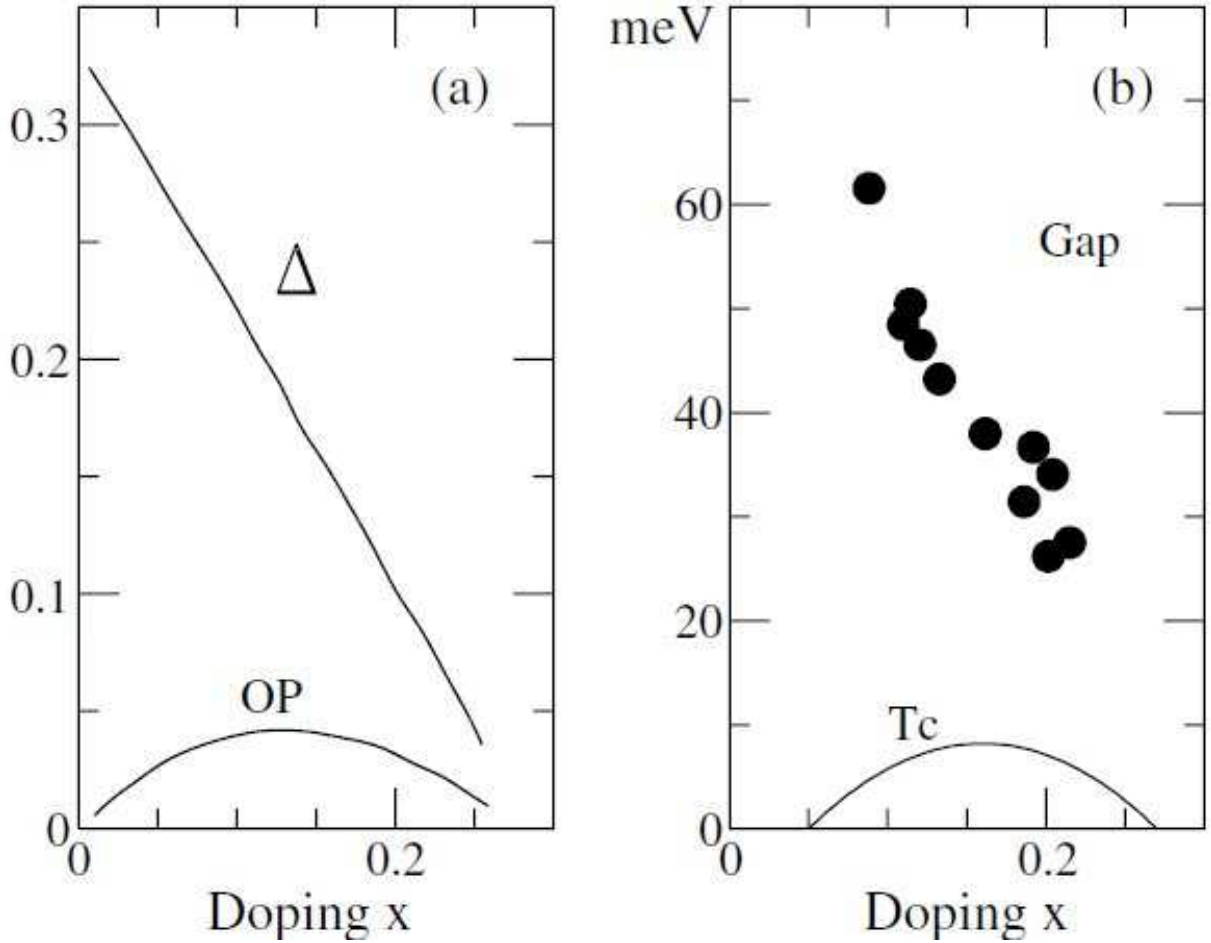
- SC order parameter

$$\Phi = \lim_{|\mathbf{r}-\mathbf{r}'|\longrightarrow\infty} F_{\alpha,\alpha}(\mathbf{r}-\mathbf{r}')$$

  Off-diagonal Long Range Order (ODLRO)

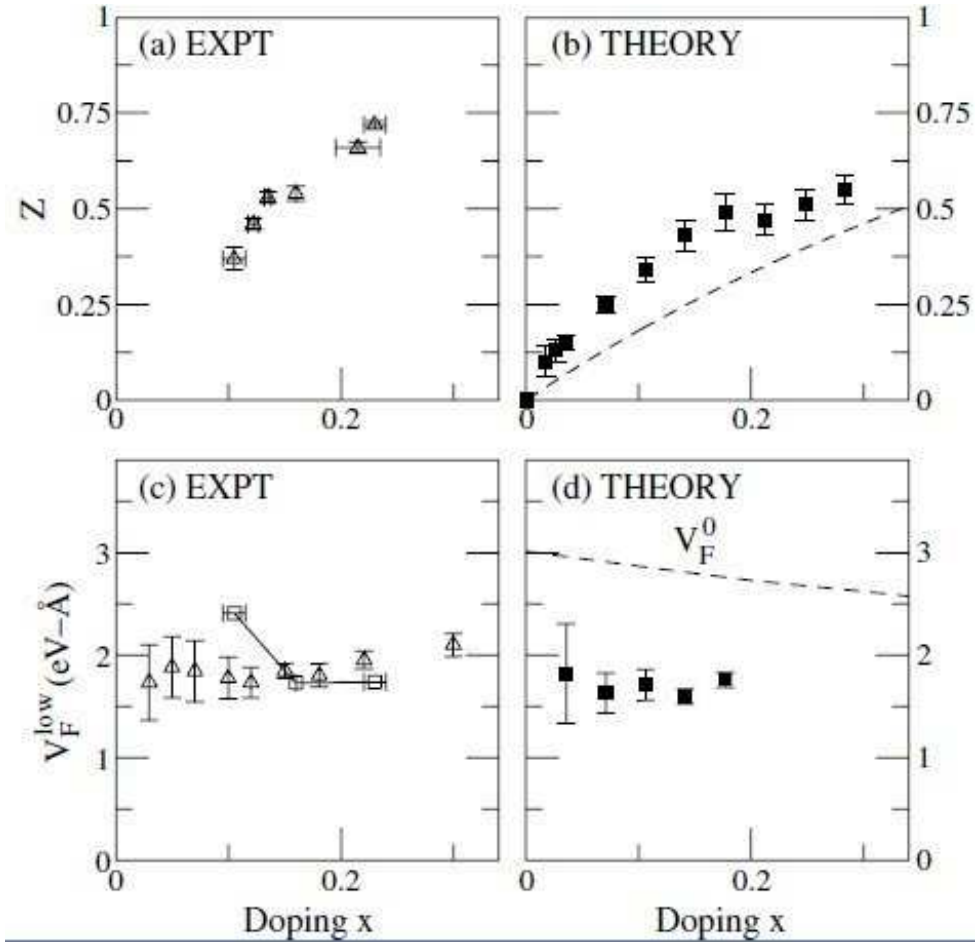
Results from Paramekanti et al.

- Calculation includes three site hopping



- Why does Φ go to zero at x?...*key result of projection*!

More results from Paramekanti et al.



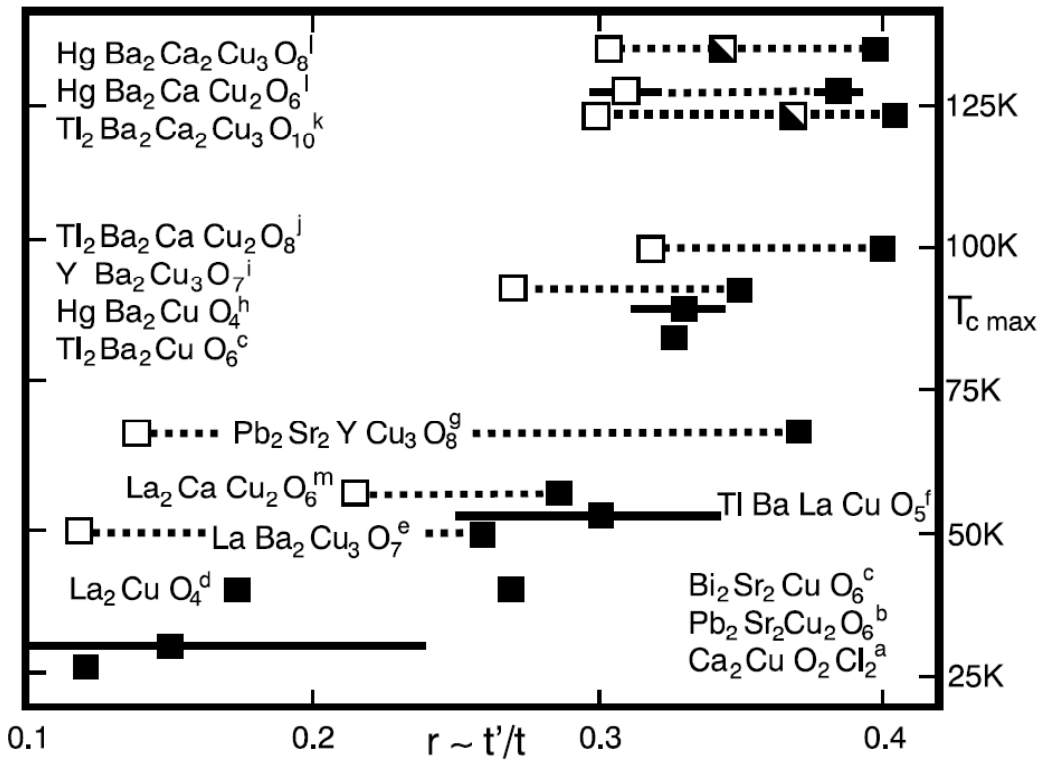
- Seems to agree qualitatively with many experiments
- What about antiferromagnetism?

Cuprates: Our Focus

- Is there a transition from antiferromagnetic ground state to a superconducting state? What is the nature of this transition? Do antiferromagnetism and superconductivity co-exist? (Previous work: Gros et al, 1988, Giamarchi et al 1990, Ogata et al, 1995, Lee et al. 1995-2003)
- What is the origin of the electron-hole asymmetry? Why does electron doping "protect" the antiferromagnetic state?
- What energy scales determine the answers to the above questions? Does the next-near neighbour and third-near neighbour hopping affect the ground state and the transition? How?
- There is a suggestion (Pavarini et al., PRL, 2001)) based on the results of first principles calculations that T_c^{max} is correlated with the ratio of the second neighbour hopping to that of the nearest neighbour hopping? What is the microscopic reason behind this?
- Is there a "single parameter" description of the phase diagram that captures the "material dependencies"?

Material Dependence of T_c^{max}

- Range parameter $r = t'/t$, $t'' = t'/2$ (Pavarini et al., 2001)



- Correlation between T_c^{max} and r, r obtained from *ab initio* electronic structure methods

Meanfield Theory

- Meanfield breakup up of $\mathbf{S}_i \cdot \mathbf{S}_j = \left(c^\dagger_{i\alpha} \frac{1}{2} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta} \right) \cdot \left(c^\dagger_{j\alpha'} \frac{1}{2} \boldsymbol{\sigma}_{\alpha'\beta'} c_{j\beta'} \right)$
- Neel channel

$$\mathbf{S}_i \cdot \mathbf{S}_j \sim \langle \mathbf{S}_i \rangle \mathbf{S}_j + ...$$

  with $\langle \mathbf{S}_i \rangle = m_N \mathbf{e}_z e^{i\mathbf{R}_i \cdot \mathbf{Q}}, \mathbf{Q} = (\pi, \pi)$
- d-wave channel

$$\mathbf{S}_i \cdot \mathbf{S}_j \sim \Delta_{ij} \left(c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{j\uparrow} \right) + ...$$

  with $\Delta_{ij} = \Delta$ on x-bonds and $\Delta_{ij} = -\Delta$ on y-bonds
- "Fock"-channel

$$\mathbf{S}_i \cdot \mathbf{S}_j \sim \chi_{ij} c^\dagger_{i\sigma} c_{j\sigma} + ...$$

  with $\chi_{ij} = \chi', \chi''$ ... "renormalizes" kinetic energy
- Four "molecular field parameters": m_N, Δ, χ', χ''

Meanfield Theory

- Mean field Hamiltonian

$$\begin{aligned}\mathcal{H}_{MF} &= \sum_{\mathbf{k},\sigma} \xi(\mathbf{k}) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\ &+ \frac{1}{2} \sum_{\mathbf{k}} \Delta(\mathbf{k}) \left(c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + \text{h. c.} \right) \\ &+ \frac{1}{2} \sum_{\mathbf{k}\sigma} \sigma m_N J(\mathbf{Q}) c^{\dagger}_{\mathbf{k}+\mathbf{Q},\sigma} c_{\mathbf{k}\sigma}\end{aligned}$$

  contains *five parameters* $\{\chi', \chi'', \Delta, m_N, \mu\}$ – gives the "one particle" states

- Δ: Gap parameter
- m_N: Neel order parameter
- μ: Hartree shift
- χ', χ'' : Fock shifts

Variational Ground State Construction

- Constructed in two steps
  - Diagonalize the Hamiltonian *without* the paring term...give rises to two SDW bands $d^\dagger_{\mathbf{k}\alpha}$ which disperse as $E_\alpha(\mathbf{k})$
  - Introduce pairing in the two spin split bands...no "cross pairing" terms arise
- Construct a BCS wavefunction

$$|\Psi\rangle = \prod_{\mathbf{k}\alpha}(u_{\mathbf{k}\alpha} + v_{\mathbf{k}\alpha} d^\dagger_{\mathbf{k}\alpha\uparrow} d^\dagger_{-\mathbf{k}\alpha\downarrow})|0\rangle, \quad \frac{v_{\mathbf{k}\alpha}}{u_{\mathbf{k}\alpha}} = (-1)^{\alpha-1} \frac{\Delta(\mathbf{k})}{E_\alpha(\mathbf{k}) + \sqrt{E^2_\alpha(\mathbf{k}) + \Delta^2(\mathbf{k})}}, \quad \alpha = 1, 2$$

- Project to N particle subspace

$$|\Psi\rangle_N = \left(\sum_{i,j} \varphi(\mathbf{R}_{i\uparrow}, \mathbf{R}_{j\downarrow}) c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} \right)^{N/2} |0\rangle$$

- The "pairing function" $\varphi(\mathbf{R}_i, \mathbf{R}_j)$ is determined by the parameters m_N, Δ...

Electron Doping

- Electron doped Hamiltonian is obtained by a particle-hole transformation (Lee et al. 1997, 2003, 2004)
- $c^\dagger \longrightarrow c$ on A sublattice, $c^\dagger \longrightarrow -c$ on B sublattice
- Corresponds to $t \longrightarrow t$, $t' \longrightarrow -t'$, $t'' \longrightarrow -t''$
- Choose sign convention such that holed doped side has all ts positive...electron doped side will have t' and t'' negative...

What do we measure?

- Staggered magnetization

$$M = \frac{2}{N}\langle \sum_{i\ \epsilon A} S_i^z - \sum_{i\ \epsilon B} S_i^z \rangle$$

- The superconducting correlation function (Paramekanti et al. 2004)

$$F_{\alpha,\beta}(\mathbf{r}-\mathbf{r}') = \langle B^\dagger_{\mathbf{r}\alpha} B_{\mathbf{r}'\beta} \rangle$$

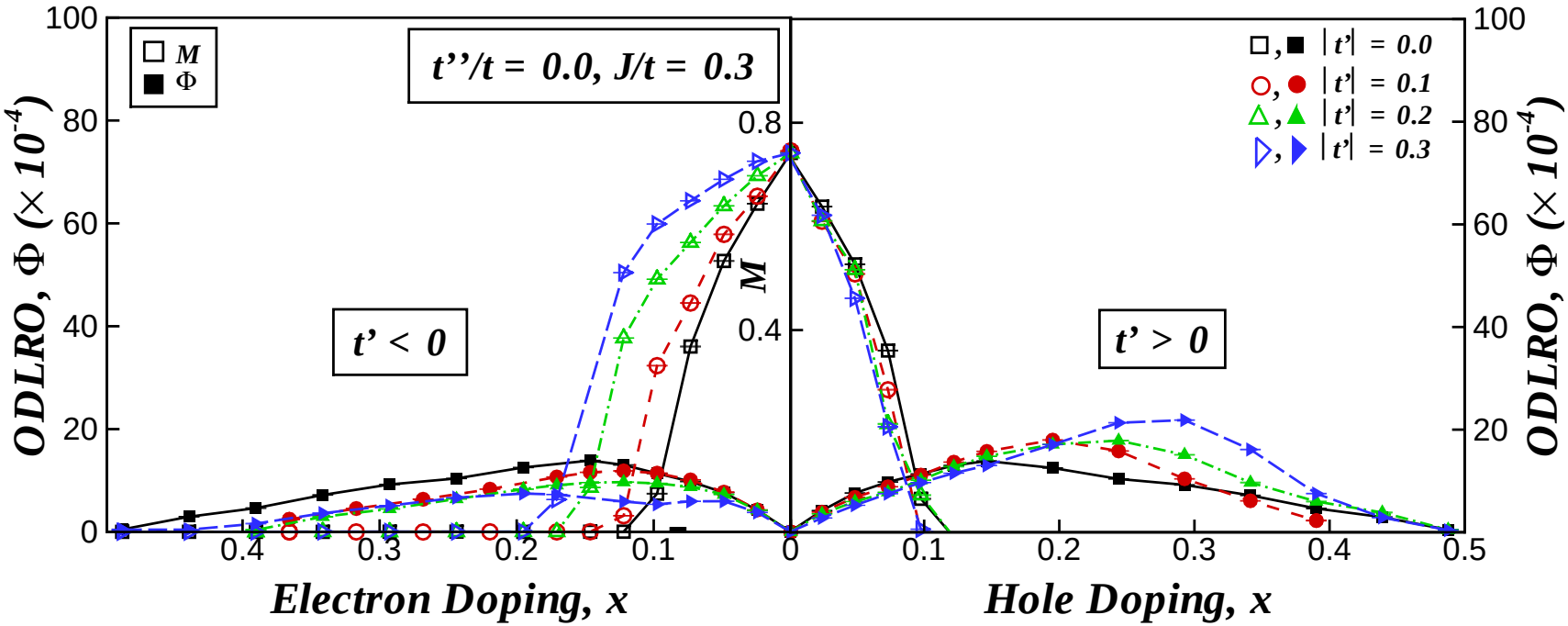
$B^\dagger_{\mathbf{r}\alpha} = \frac{1}{2}(c^\dagger_{\mathbf{r}\uparrow} c^\dagger_{\mathbf{r}+\hat{\alpha}\downarrow} - c^\dagger_{\mathbf{r}\downarrow} c^\dagger_{\mathbf{r}+\hat{\alpha}\uparrow})$ creates a singlet on the bond $(\mathbf{r}, \mathbf{r}+\hat{\alpha})$, $\alpha = x, y$

- SC order parameter

$$\Phi = \lim_{|\mathbf{r}-\mathbf{r}'|\longrightarrow\infty} F_{\alpha,\alpha}(\mathbf{r}-\mathbf{r}')$$

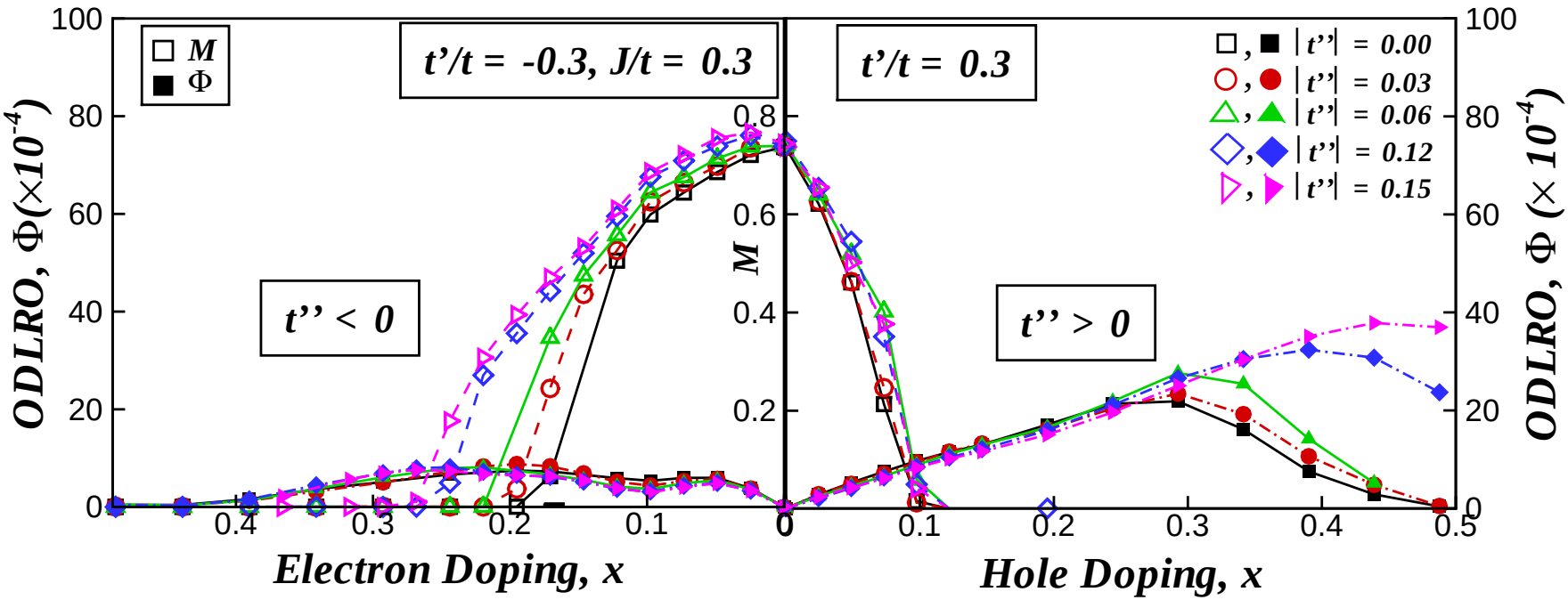
Off-diagonal Long Range Order (ODLRO)

Phase Diagram ($t'' = 0$)



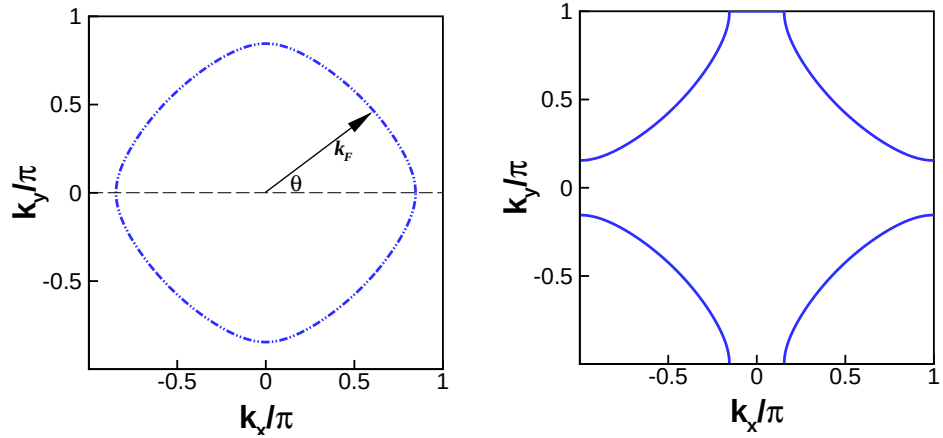
- SC and AF coexist on both h and e doped systems
- With increasing $|t'|$, SC enhanced on h doped side, AF on the e doped side ((Lee et al, 2004, Trambley et al, 2006, Kotliar et al 2007))
- New result: $|t'|$ does not affect x_{AF} on the hole doped side, and slightly "weakens" SC on the e doped side

Phase Diagram ($t'' \neq 0$)



- h-doped: Increasing $|t''|$ *enhances* SC, x_{AF} is unaffected
- e-doped: Increasing $|t''|$ *enhances* AF, SC is unaffected
- ...
- Is there a "single parameter" characterization...a unified picture?

Fermi Surface Convexity Parameter η

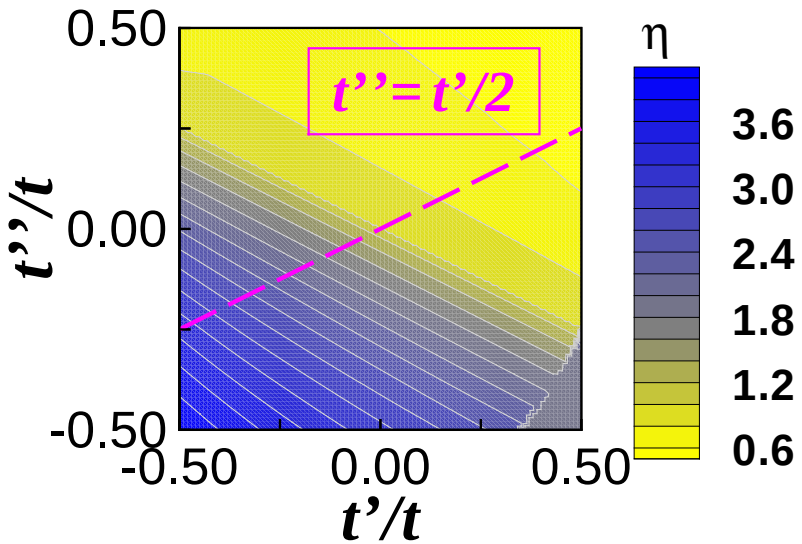


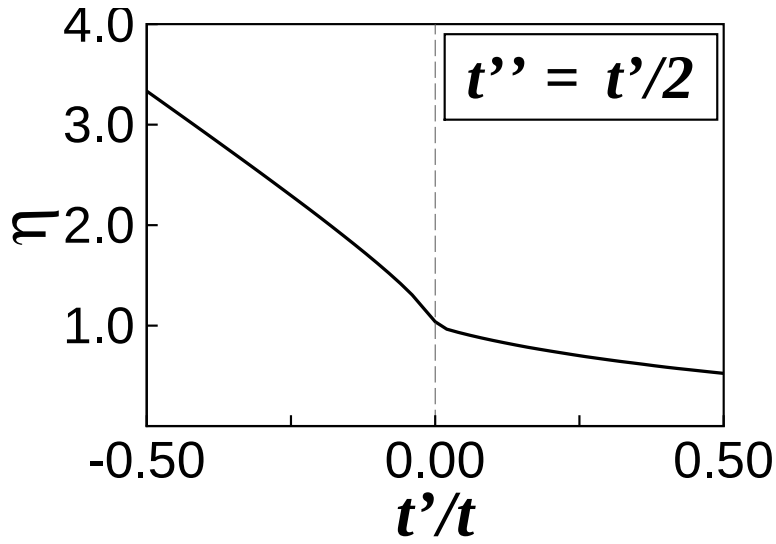
- Bare Fermi surface (BFS) at zero doping
- Fermi surface convexity parameter

$$\eta = 2\left(\frac{k_F^{\text{NODE}}}{k_F^{\text{ANTINODE}}}\right)^2$$

- $\eta = 1$ when $t' = t'' = 0$
- $\eta > 1$ convex BFS, $\eta < 1$ concave BFS
- Claim: "Everything" is determined by η (for given t and J); Convex BFS encourages AF, concave BFS promotes SC!

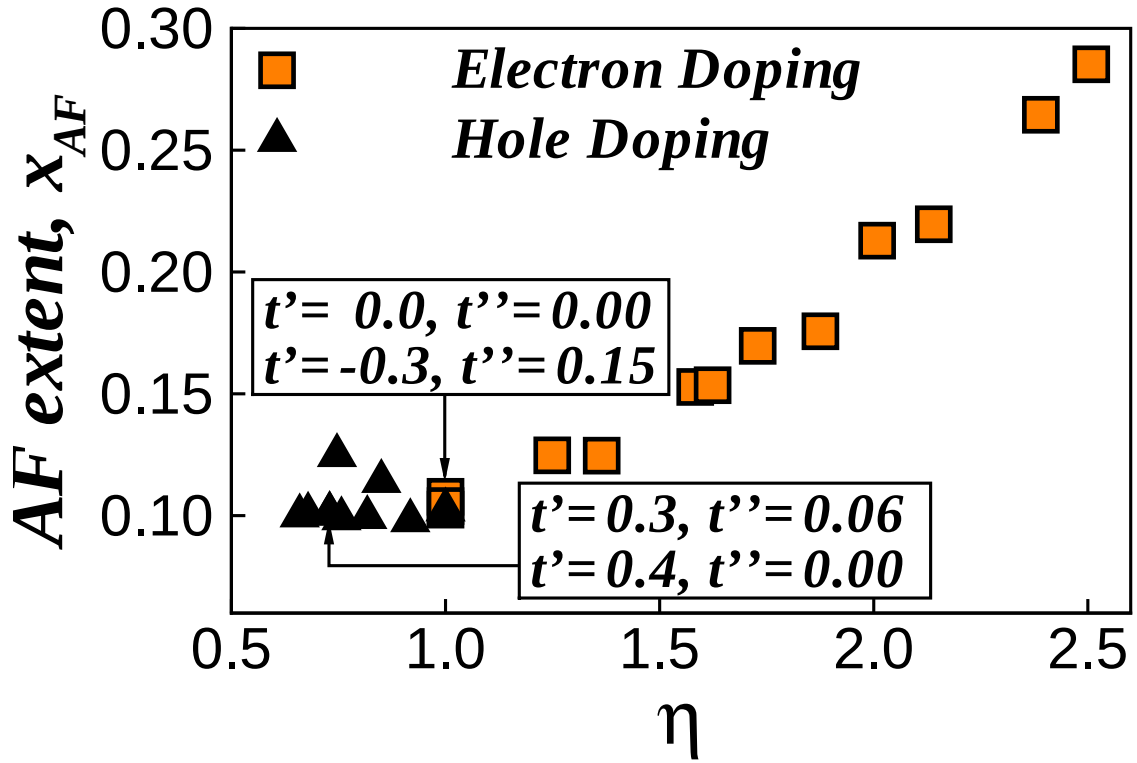
Fermi Surface Convexity Parameter η





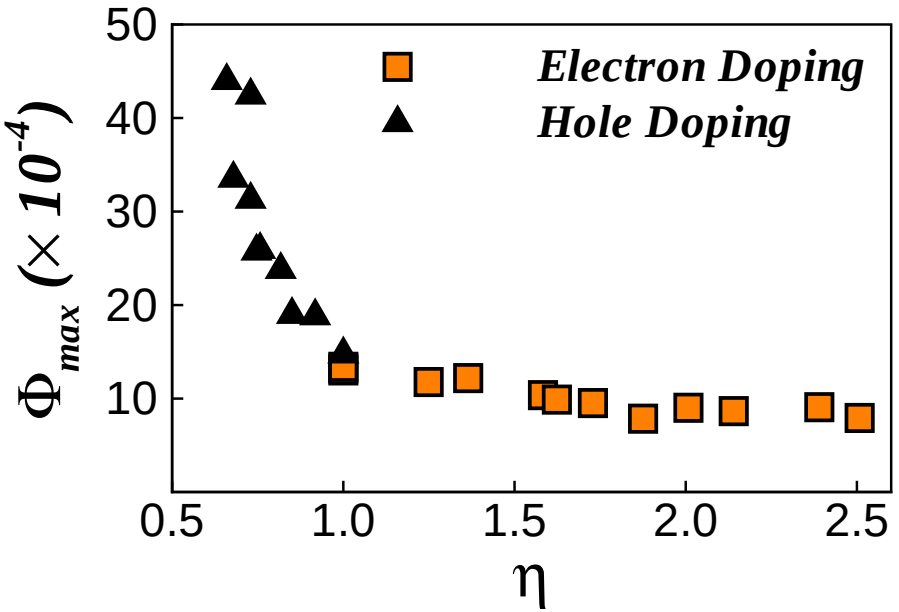
- $\eta > 1$ convex BFS, $\eta < 1$ concave BFS
- For $t'' = t'/2$: η is *monotonically* related to range parameter of Pavarini et al.!
- Valid for $t'' \neq t'/2$

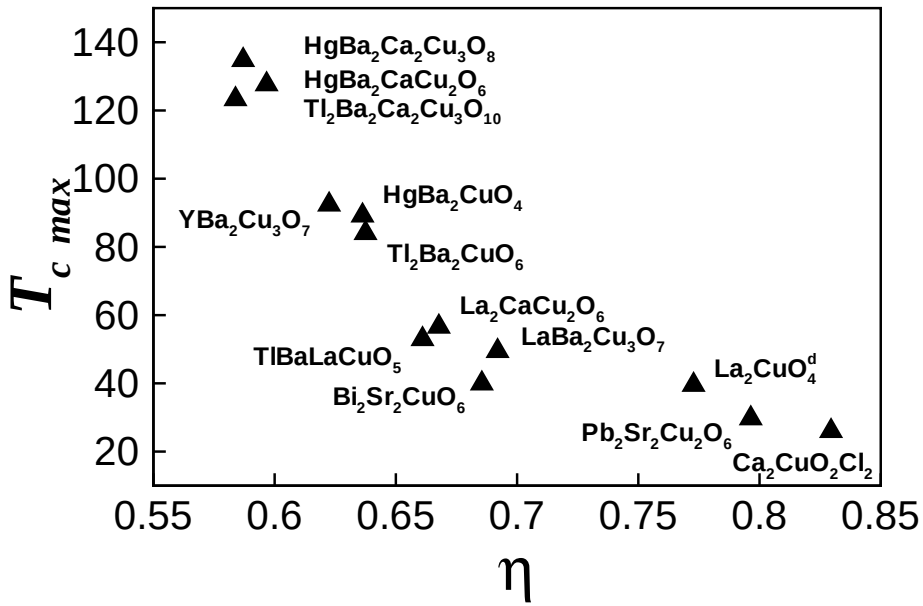
"Extent" of antiferromagnetism x_{AF} and η



- Convex BFS promote AF, x_{AF} increases linearly with η!
- Different values of t', t'' with same η fall on top of each other!

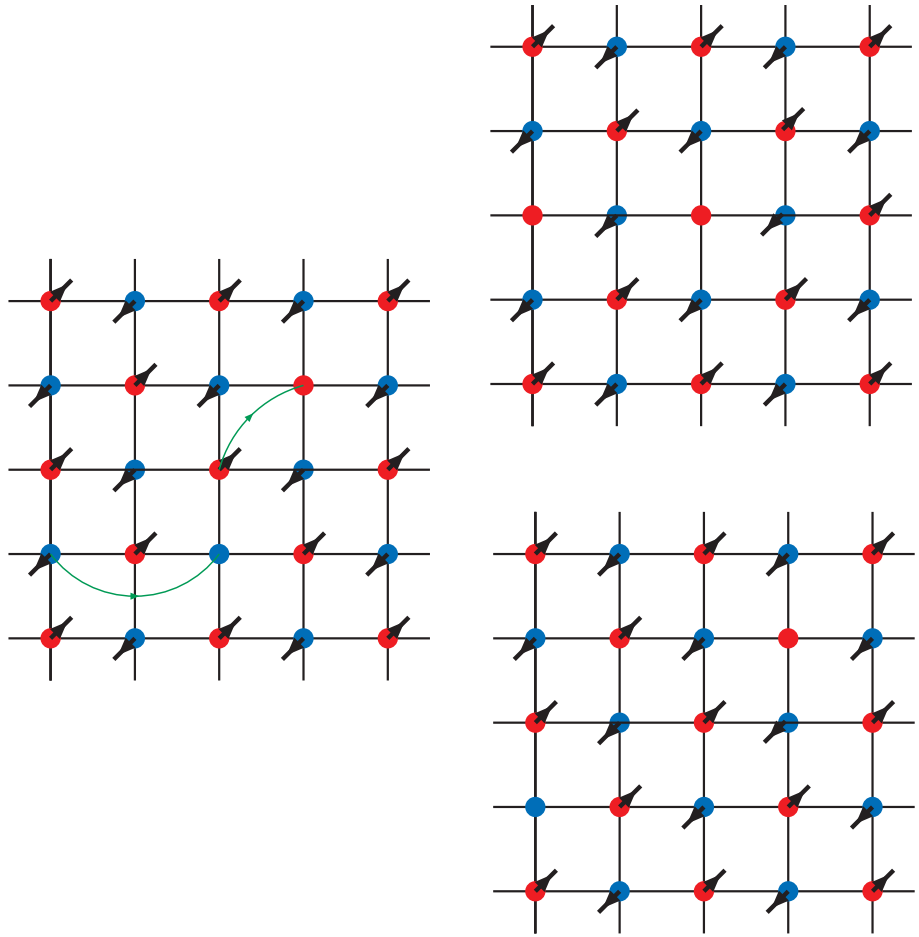
Optimal ODLRO Φ_{max} and η





- The maximum ODLRO (Φ_{max}) is promoted by a *concave* BFS
- Φ_{max} taken to be a measure of T_c, suggests η "determines" T_c!
- Consistent with experiments, Pavarini et al., 2001

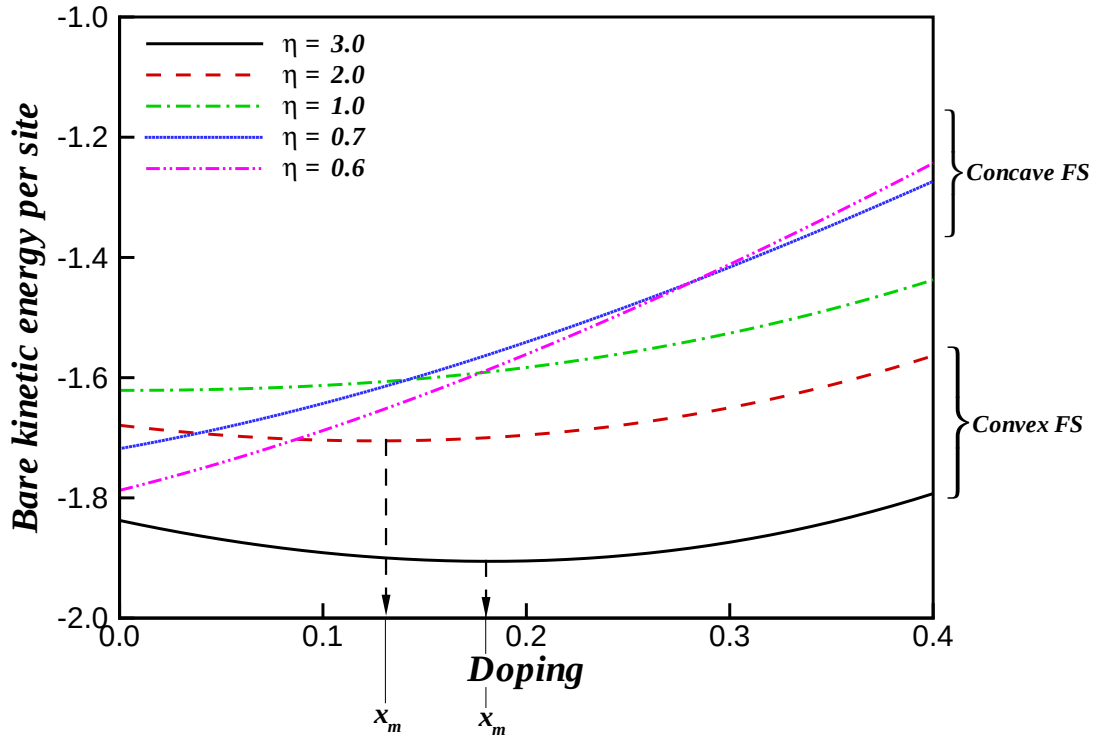
Physics of η



- Key (well known) point: t' and t'' do not disturb the AF background
- Question: Do t', t'' help *gain* kinetic energy?

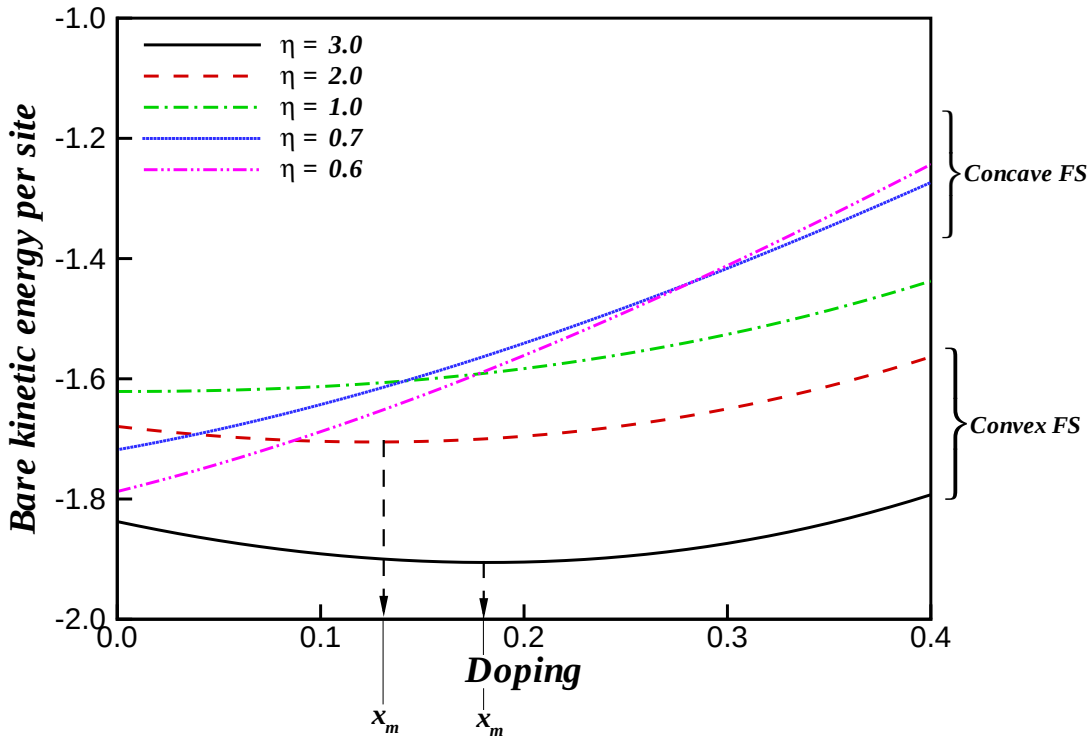
Physics of η

- Not always! Look at the *bare* kinetic energy as fn. of doping



- For $\eta > 1$, the bare KE *falls* with increasing doping, attains a minimum at x_m^{BKE}
- x_m^{BKE} increases with η
- This *gain* in KE arises from t', t'' and hence AF will be stable until x_m^{BKE}...explains why x_{AF} increases with η!

Physics of η



- For $\eta < 1$, the bare KE monotonically increases with doping...greater rate of increase of BKE for more concave FS...
- Plausible that SC is stabilized in this case...both KE and exchange energies are happy!

Summary

What is done

- VMC of $t - t' - t'' - J$ model...a detailed study of material dependencies
- An efficient method for optimizing variational wavefunctions

What is learnt

- Cuprate phase diagram is characterized by a single parameter...η (for given t and J)
- Difference between hole and electron doping
- Microscopic origin of Pavarini et al. relation
- Suggestion to increase T_c: Make BFS more concave!

Reference

S. Pathak, V. B. Shenoy, M. Randeria, N. Trivedi, *Phys. Rev. Lett.* **102**, 027002 (2009)

Graphene: Superconductor?

Work done in collaboration with G. Baskaran

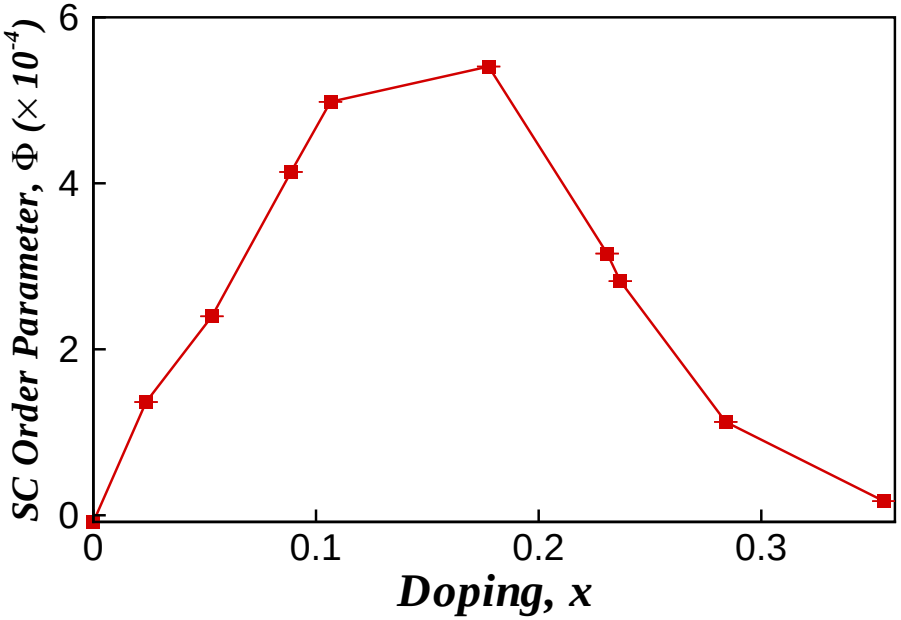
- Graphene - many benzene's connected togather
- Pauling's idea of resonance
- Graphene: Correlated or not?
- Experiments suggest a $U/t \sim 2.4$
- *Not* strongly correlated

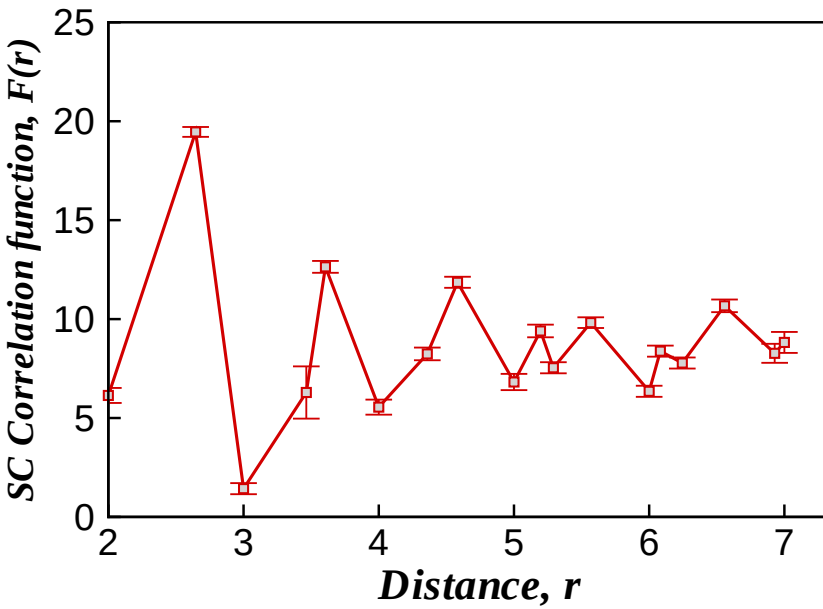
Graphene Superconductivity

- Singlet formation tendency...J (difference between singlet triplet energies)
- Undoped graphene has zero density of states...MFT suggests that a critical J is required to induce SC
- J in graphene is *lower* than the critical value, undoped graphene is not a SC
- What about doped graphene?
- Meanfield theory of Black-Schaffer suggested a $d + id$ state

Graphene Superconductivity: VMC Results

- $|\Psi\rangle = g^D |BCS_{d+id}\rangle$





- Optimum doping around $x \sim 0.15$
- Agrees with other works e.g., Honerkamp, *PRL* (2008)