Variational Monte Carlo Method for Fermions

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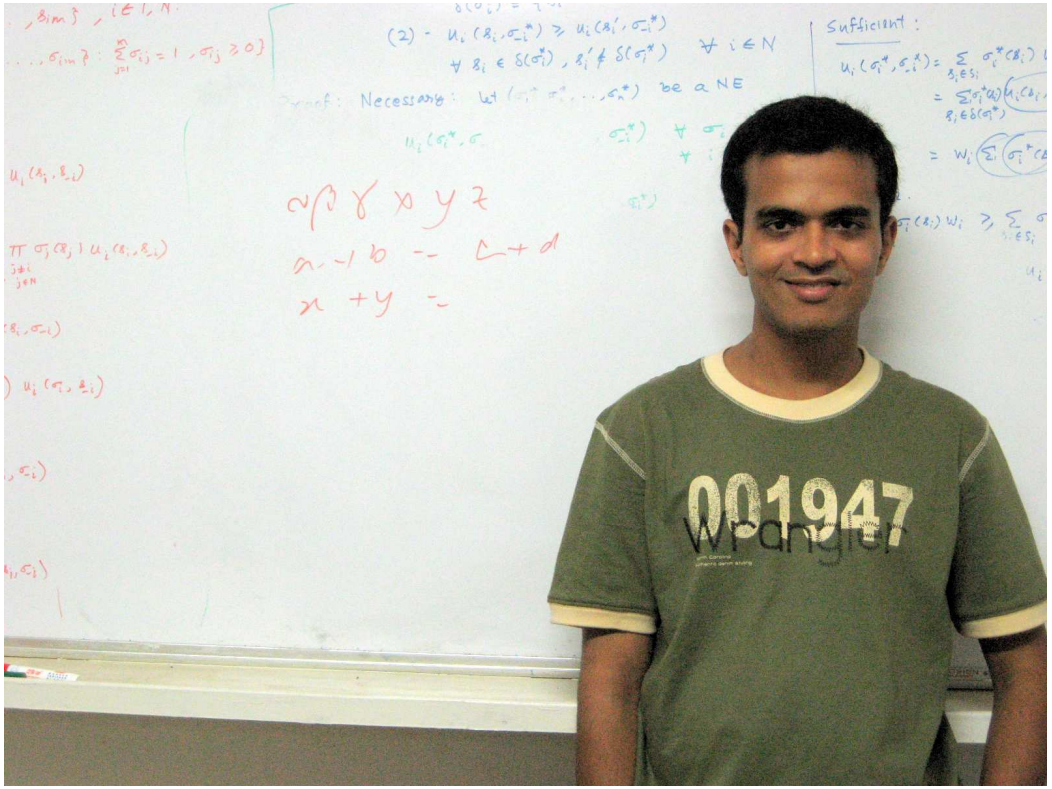
Indian Institute of Science, Bangalore

Mahabaleswar, December 2009

Acknowledgements



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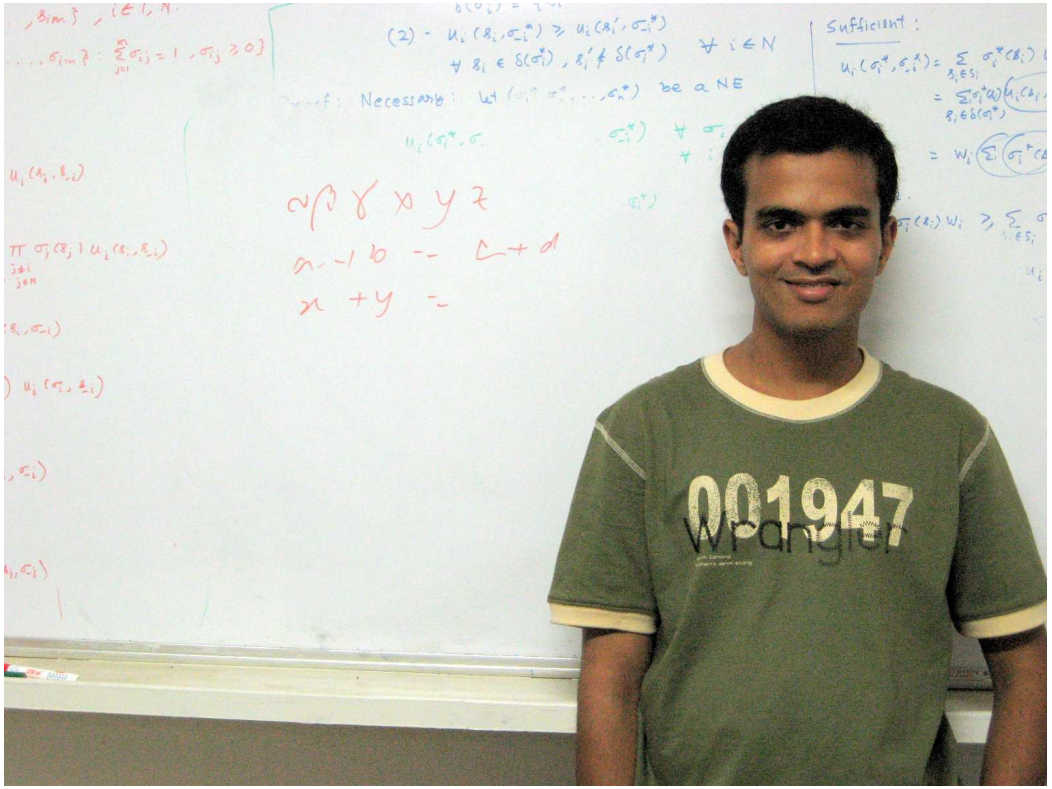

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- Department of Science and Technology

Plan of the Lectures on Variational Monte Carlo Method

- Motivation, Overview and Key Ideas (Lecture 1, VBS)

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The Strongly Correlated Panorama...

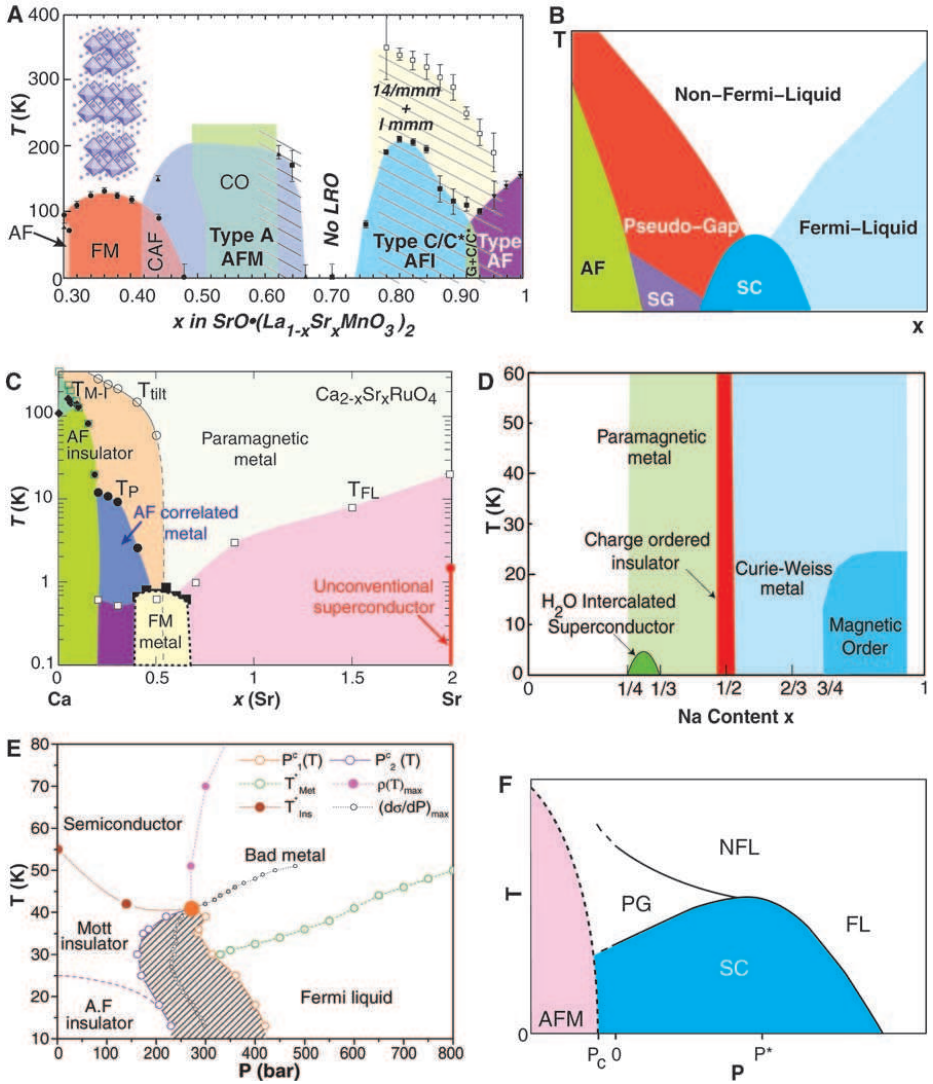
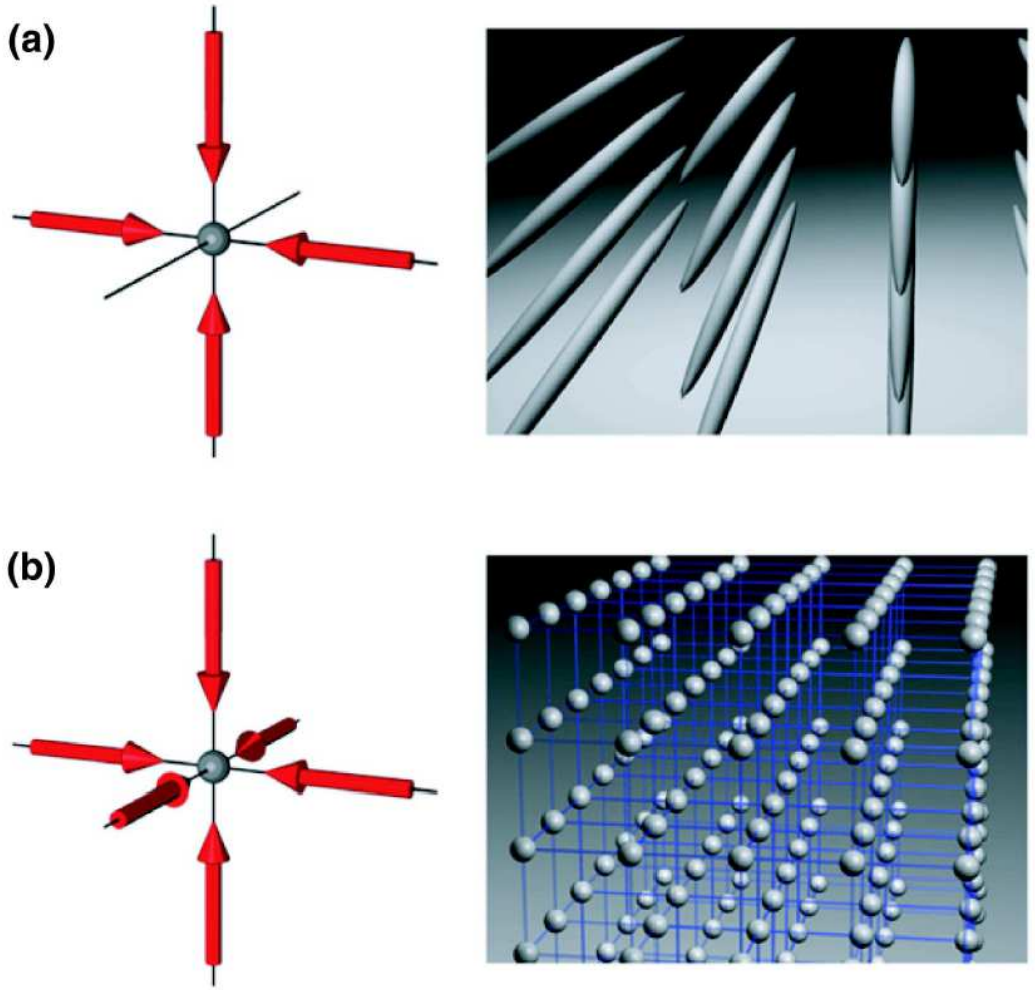


Fig. 1. Phase diagrams of representative materials of the strongly correlated electron family (notations are standard and details can be found in the original references). **(A)** Temperature versus hole density phase diagram of bilayer manganites (*74*), including several types of antiferromagnetic (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?

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- Nature(Science)/Nature Physics/PRL/PRB...

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- Ceperley, Chester and Kalos, *PRB* **17**, 3081 (1977)

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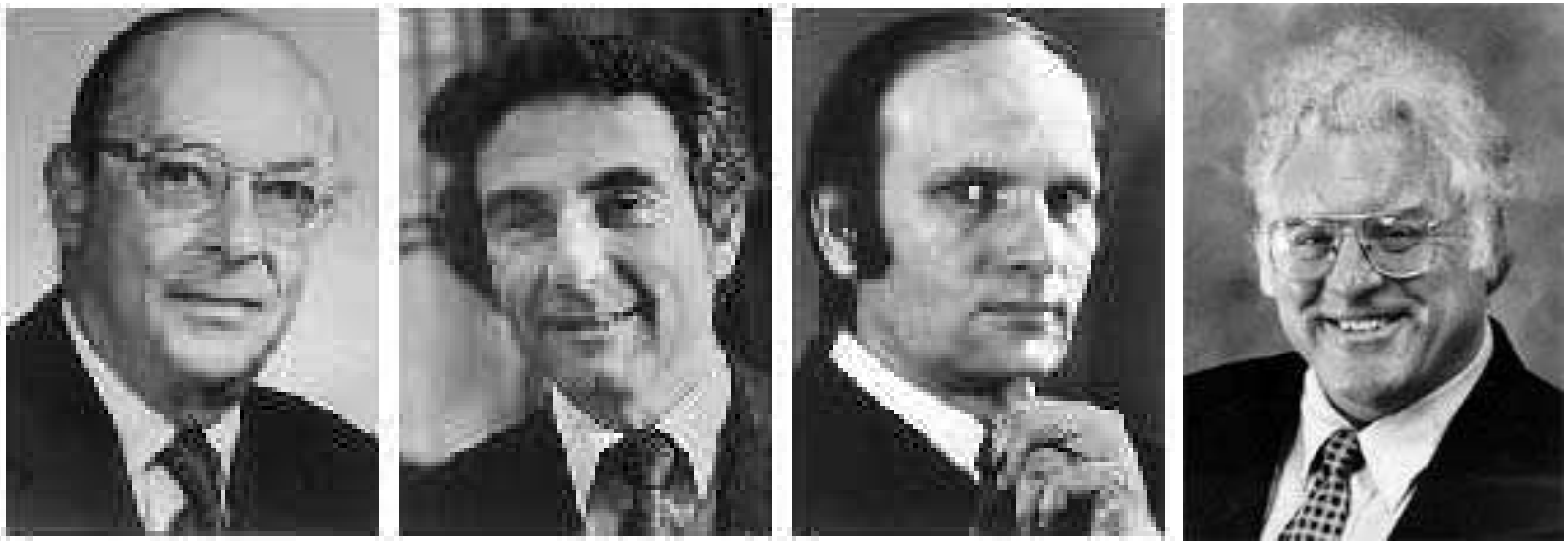

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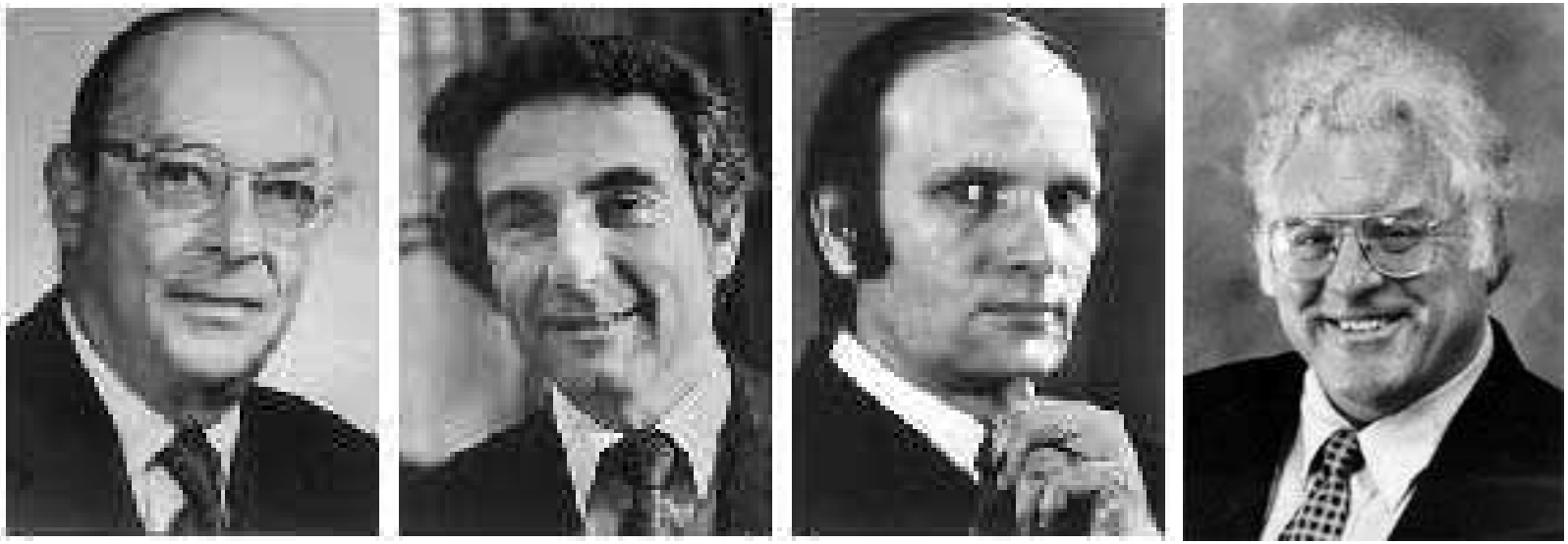

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$$H|\Psi\rangle = E|\Psi\rangle$$

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  - The state(s) that minimises(minimise) $E[\Phi]$ is(are) the ground state(s)

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- Example shows key ideas (*and limitations*) of the variational approach!

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- ...your guess is *not* as *good* as mine!

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- Usually MFT provides us with intuitive starting point...we can then "well design" the variational wavefunction to include the fluctuations that we miss

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- 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

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- Now,

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

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- Note that in most practical cases we need sum the denominator as well, since we use *unnormalized* wavefunctions!

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- Solution...use Monte Carlo method to perform the sum!

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- 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 $C_1, C_2 ... C_m ...$ etc; we will use $P(1) \equiv P(C_1)$, and in general $P(m) \equiv P(C_m)$ and $\sum_C \equiv \sum_m$

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- 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 $\mathbb{P}(t+1)$?

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

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- 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

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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"

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- Let us suppose that we have "designed" a suggestion probability matrix...what is the acceptance probability matrix?

Acceptance Matrix

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

Acceptance Matrix: Popular Choices

- Metropolis

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

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- Heat Bath

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

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- 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

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- 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

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

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- 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 do 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 $\mathbb{P}$ and *project out* the ground state $\mathbb{P}_{GroundState}$ by repeated application of $\mathbb{W}$

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- ...all is *not* lost!

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- 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* l, r_l *and* r'_l; written in terms of matrices

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

and

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

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

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- 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, agian, appears to be $O(N^3)$!

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- On acceptance of the suggested configuration, we need to compute Φ^{-1} which will be the new Ψ^{-1} for the next step

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- In short VMC, at its best, is $O(N^2)$ hard! Note that calculation of correlation functions can be harder

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