TRIAL MANY BODY WAVE FUNCTION

$$\Psi_T(r_1, r_2, \ldots r_N) \equiv \Psi(R)$$

$$\left\langle \hat{O} \right\rangle = \frac{\left\langle \Psi_T \,|\, \hat{O} \,|\, \Psi_T \right\rangle}{\left\langle \Psi_T \,|\, \Psi_T \right\rangle} = \frac{\sum_R |\Psi_T(R)|^2 \, O(R)}{\sum_R |\Psi_T(R)|^2} = \sum_R P(R) O(R)$$

Many interacting particles

Multi dimensional integrals

Classical Stat Mech

$$H = -J\sum_{<ij>} S_i S_j \qquad S_i = \pm 1$$

N sites: each site can be $\uparrow$ or $\downarrow$ $= 2^N$ configurations

$$Z = Tre^{-\beta H} = \sum_{\{C\}} e^{-\beta E(C)}$$

$$E = \frac{1}{Z}\sum_{\{C\}} e^{-\beta E(C)} E(c)$$

HOW CAN WE EVALUATE MULTIDIMENSIONAL INTEGRALS??

USE MONTE CARLO METHODS

Evaluating Multi-dimensional integrals

Speed

Monte Carlo is an efficient way to evaluate integrals
For large numbers of dof

Quadrature method: 10 divisions
Nparticles=8 dimensions d=2

Evaluate integrand at 10^{2*8} points

Computation speed= 10 MFLOPS = 10^7 Evaluations/sec

Integrand evaluation takes~10^9 sec~40years

Monte Carlo < 1 minute for 1% accuracy

ACCURACY

# of points at which integrand evaluated=M
degrees of freedom=f=d* Nparticles
Error:

$$\sigma_{quad} \sim M^{-2/f}$$

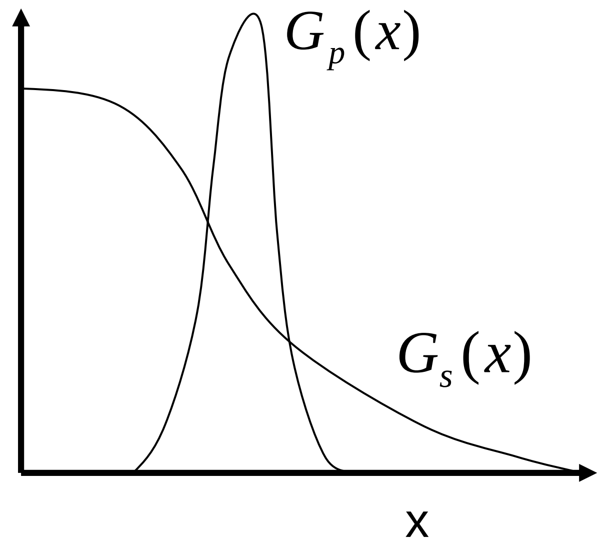
$$\sigma_{MC} \sim M^{-1/2}$$

MC more efficient for $f = dN \geq 4$

Evaluating integrals

$$I = \int_0^1 dx f(x) = \int_0^1 dx G_p(x) G_s(x)$$

$$G(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{\frac{-(x-a)^2}{2\sigma^2}}$$



Monte Carlo I:
(a) Pick x at random in the range [0,1]
(b) Evaluate

$$f(x) = G_p(x) G_s(x)$$

at the randomly picked x

$$I = \sum_{x_i} f(x_i)$$

CODES PROVIDED

Exact result: exact.f
Quadrature method: quad.f
Monte Carlo I: mc1.f
Monte Carlo II: mc2.f
(with importance sampling)

Monte Carlo II with importance sampling

a) Pick x with probability $G_p(x)$ which is sharply peaked

b) Make a list of points $X = \{x_1, x_2, \ldots x_M\}$
such that the probability of finding a particular x_i in this set $P(x_i) = G_p(x_i)$

$$I = \sum_{x \in X} G_s(x)$$

How to make such a list? METROPOLIS ALGORITHM

Computational Physics
Koonin, Addison-Wesley

Start with some initial x
Let W(x,x') be a transition probability or a rule which takes x-→ x'

W(x,x') must satisfy:

$$W(x \to x') \geq 0$$

$$\sum_{x'} W(x \to x') = 1$$

$$P(x') = \sum_{x} P(x) W(x \to x')$$

Ergodicity: must be able to access all phase space

DETAILED BALANCE

$$P(x)W(x \to x') = P(x')W(x' \to x)$$

METROPOLIS ALGORITHM

Is one algorithm that imposes detailed balance

$$W(x \rightarrow x') = \min(1, \frac{P(x')}{P(x)})$$

Operationally

1. Pick a starting point x_0
2. Evaluate $P(x_0)$
3. Choose x_{trial} at random
4. Evlaluate $P(x_{trial})$
5. If $\dfrac{P(x_{trial})}{P(x_0)} \geq r$ (random number [0,1])

   put $x_1 = x_{trial}$ and put x_1 in the list X
6. If $\dfrac{P(x_{trial})}{P(x_0)} < r$ put $x_1 = x_0$ and put x_1 in the list X

$$I = \int_0^1 dx G_p(x; a_2, \sigma_2) G_s(x; a_1, \sigma_1)$$

$$G(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{\frac{-(x-a)^2}{2\sigma^2}}$$

$$a_1 = 0; \sigma_1 = 0.5$$
$$a_2 = 0.5; \sigma_2 = 0.05$$

Exact=0.48393

$$a_1 = 0; \sigma_1 = 0.5$$
$$a_2 = 0.5; \sigma_2 = 0.01$$

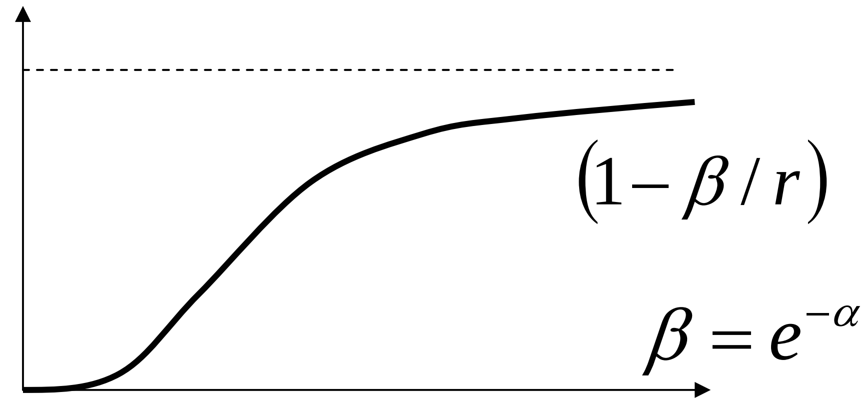
Exact=0.48393

#points	I(MC1)	error	I(MC2)	err	I(MC1)	err	I(MC2)	err
100	0.388	0.28	0.463	0.034	0.383	0.64	0.4931	0.009
1000	0.488	0.11	0.4816	0.014	0.376	0.18	0.4867	0.004
10000	0.507	0.03	0.4841	0.003	0.4977	0.09	0.4841	0.002
100000	0.4837	0.012	0.48415	0.0015	0.4799	0.018	0.4839	0.0004

MC1: without importance sampling
MC2: with imp. sampl.

boson.f

$$\Psi_T = \prod_{i<j} f$$



Long range correlations in ground state

EXPECTATION VALUES AND MONTE CARLO

$$\Psi(R) \equiv \Psi(r_1, r_2, \ldots r_N) = \prod_{i<j} f(r_{ij})$$

Many interacting particles
Multi dimensional integrals

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} = \frac{\sum_{R,R'} \langle \Psi_T | R \rangle \langle R | H | R' \rangle \langle R' | \Psi_T \rangle}{\sum_R \langle \Psi_T | \Psi_T \rangle}$$

$$E_T = \sum_R P(R) \underbrace{\sum_{R'} \langle R | H | R' \rangle \frac{\Psi_T(R')}{\Psi_T(R)}}_{\varepsilon(R)} = \sum_{R \in P(R)} \varepsilon(R)$$

Generate a list of configurations {R} with $P(R) = \dfrac{|\Psi_T(R)|^2}{\sum_R |\Psi_T(R)|^2}$

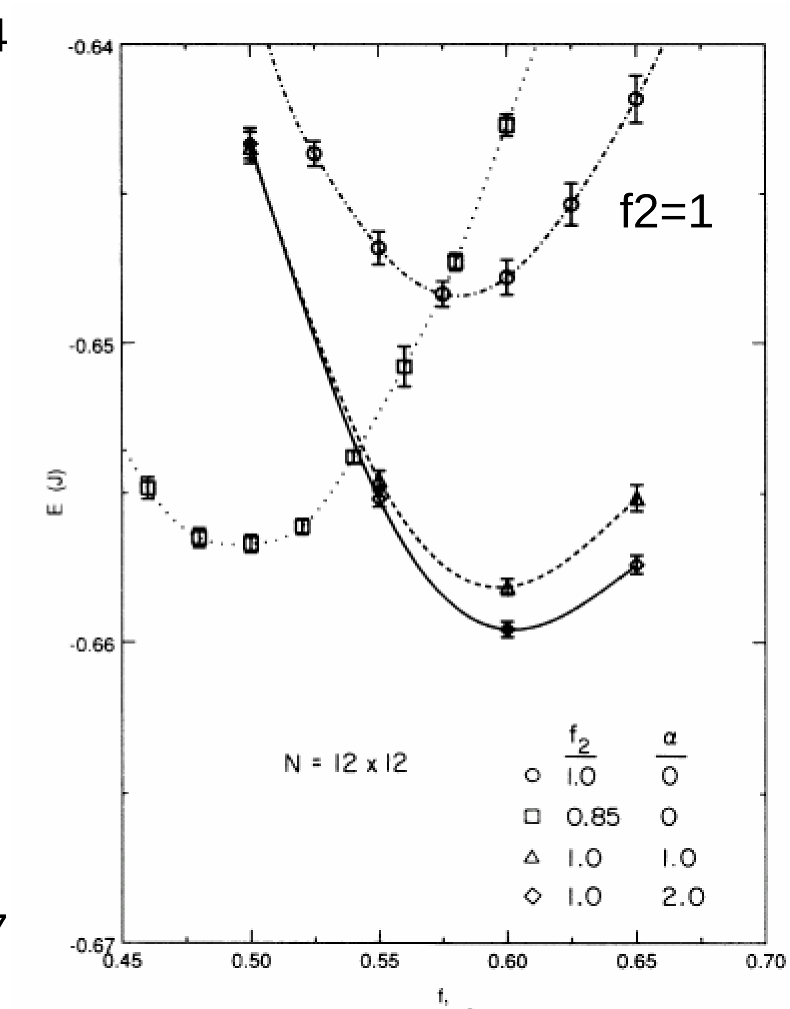
Calculate the energy $\varepsilon(R)$ In each configuration R

Eneel/NJ=-0.5

-0.64

E/NJ

-0.67



f1

NT and D.M. Ceperley
PRB 41, 4552 (1990)

GREEN FUNCTION / PROJECTOR QUANTUM MONTE CARLO

AIM: Filter out of a trial wave function the component of the true ground state

$$H\left|\Phi_\alpha\right\rangle = \varepsilon_\alpha\left|\Phi_\alpha\right\rangle$$

Exact eigenstates of H

$$\Psi_n = \left(e^{-\tau H}\right)^n \Psi_T$$

$$\Psi_n(R) = \sum_\alpha \Phi_\alpha(R) e^{-n\tau\varepsilon_\alpha}\left\langle \Phi_\alpha \middle| \Psi_T \right\rangle$$

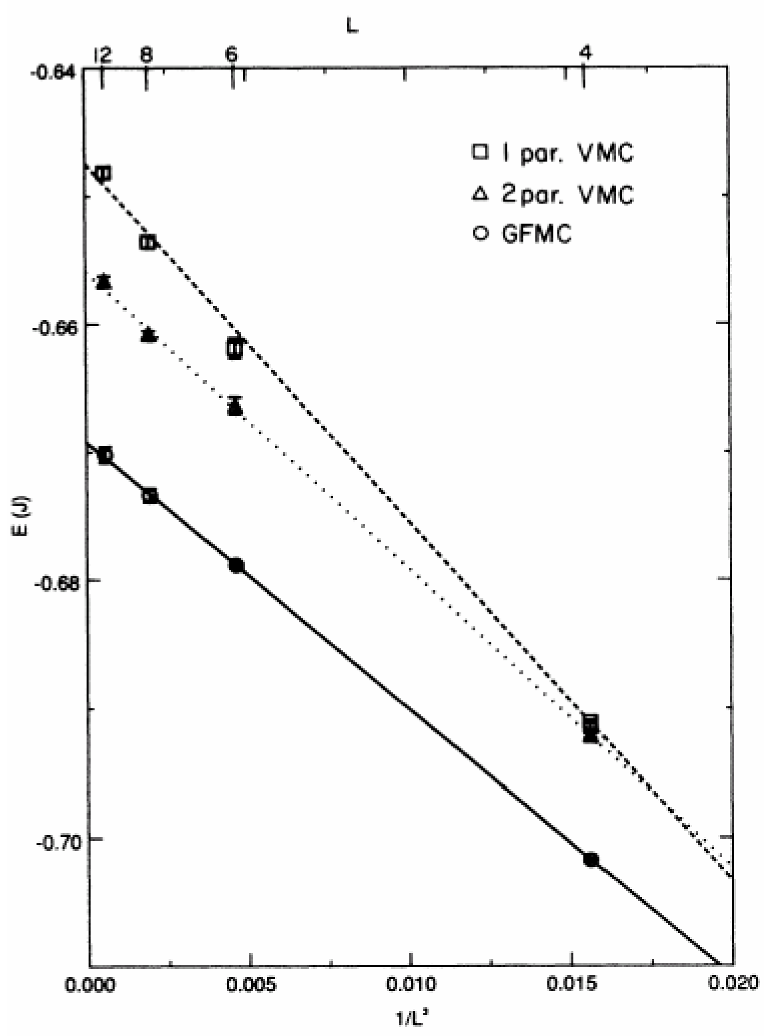
Ground state ε_0 decays most slowly

$$\underset{n\to\infty}{Lt}\, \Psi_n(R) \to \Phi_0(R)\left\langle \Phi_0 \middle| \Psi_T \right\rangle$$

$$\downarrow$$

Overlap of true ground state with trial wave function

Finite size scaling



$$E / NJ = -0.6692 \pm 0.0002$$

Best result obtained by GFMC

SUPERFLUID

MAGNET

Off diagonal long range order

$$\langle b_i^+ \rangle \neq 0$$

Magnetization in XY plane

$$\langle S_i^+ \rangle \neq 0$$

In a subspace with fixed number of particles

$$h(l) = \langle b_i^+ b_{i+l} \rangle \xrightarrow[l\to\infty]{} const \neq 0$$

$$h(l \to \infty) = \left(m_x^+\right)^2 + \left(m_y^+\right)^2$$

Condensate fraction

Sublattice magnetization in XY plane

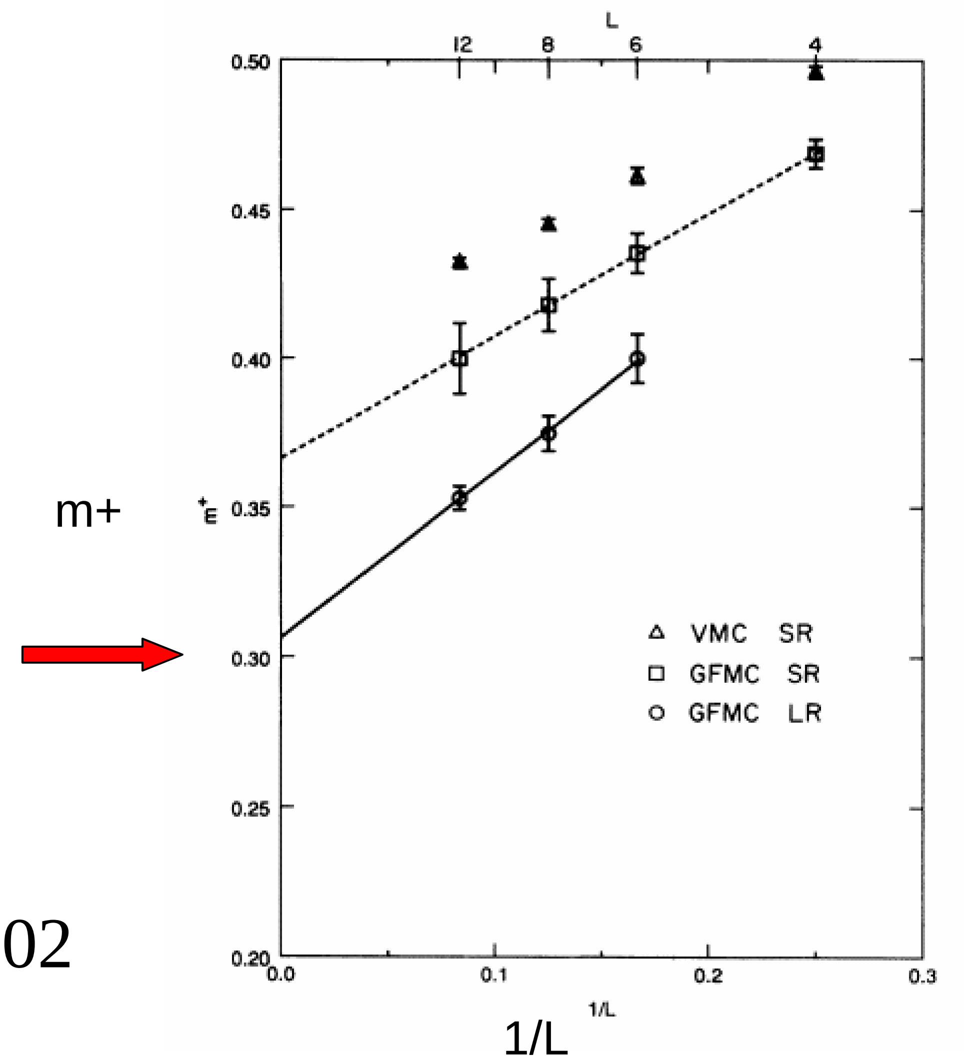
$$g(l) = \langle n_i n_{i+l} \rangle \xrightarrow[l\to\infty]{} \left(m_z^+\right)^2$$

Diagonal long range order

Sublattice magnetization along z

Staggered magnetization survives inspite of quantum fluctuations

m+



1/L

$$m^+ = 0.32 \pm 0.02$$

Quantum Monte Carlo is not one black box

Variational QMC
Green function or Diffusion QMC
Path Integral QMC
Determinantal QMC

Comparisons of the different QMC techniques

SIGN PROBLEM IN DIFFERENT INCARNATIONS

GFMC: Nodes in Wave Function

PIMC:

$$Z = \sum_{\{S\}} \det[M_{\uparrow}(\{S\})] \det[M_{\downarrow}(\{S\})] \equiv \sum_{\{S\}} P(\{S\})$$

$$\langle \hat{O} \rangle = \sum_{\{S\}} P(\{S\}) O(\{S\})$$

$$\widetilde{P} = | P |$$

$$\langle \hat{O} \rangle = \frac{\langle O \, \mathrm{sgn}(\widetilde{P}) \rangle_{\widetilde{P}}}{\langle \mathrm{sgn}(\widetilde{P}) \rangle_{\widetilde{P}}}$$

small average sign at low T leads to large fluctuations in MC averages

Recent progress: Projected techniques + Det QMC: Imada; Shiwei Zhang

Energy is sensitive only to short range correlations in wave function

For an improved description must include contribution from
zero point motion of elementary
excitations in the ground state

$$H_{ZP} = \frac{1}{2}\sum_{q<q_c} m_q(\dot{\rho}_q\dot{\rho}_{-q} + \omega_q^2\rho_q\rho_{-q})$$

$$\Psi_{ZP} = \prod_{q<q_c}\exp(-\frac{1}{2}m_q\omega_q\rho_q\rho_{-q}) = \prod_{i<j}\exp(-\frac{\alpha}{|\vec{r}_i - \vec{r}_j|})$$

$$\rho_q = \frac{1}{N}\sum_i e^{i\vec{q}\cdot\vec{r}_i}$$

$$\omega_q \sim cq$$

$$m_q \sim \frac{1}{q^2}$$

$$d = 2$$

$$\hbar c = \frac{\pi\alpha|T_k|}{2} Ja$$

My teaching philosophy is summarized in this saying by Confucius:

I hear and I forget

I see and I remember

I do and I understand