

2007 Summer School on Computational Materials Science

Quantum Monte Carlo: From Minerals and Materials to Molecules

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Reptation Monte Carlo and other topics

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Reptation Monte Carlo and other topics

OUTLINE

- Review of Diffusion Monte Carlo and Path Integral Monte Carlo
- Path Integral representation of the projector Method
- What action to use?
- How to sample paths?
- Advantages and disadvantages
- Excited states and MaxEnt(?)

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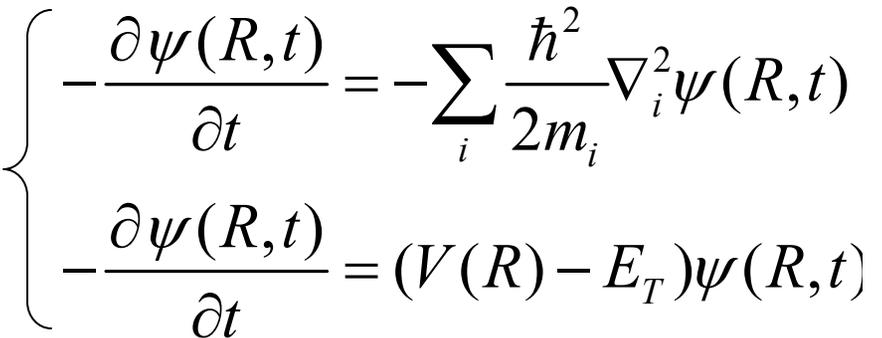
Diffusion Monte Carlo process

- Imaginary time SE.
- This is a diffusion + branching process.
- Justify in terms of Trotter's theorem.

Requires interpretation of the wavefunction as a probability density.

$$-\frac{\partial \psi(R,t)}{\partial t} = (H - E_T)\psi(R,t)$$

$$H = -\sum_i \frac{\hbar^2}{2m_i} \nabla_i^2 + V(R)$$


$$\left\{ \begin{array}{l} -\frac{\partial \psi(R,t)}{\partial t} = -\sum_i \frac{\hbar^2}{2m_i} \nabla_i^2 \psi(R,t) \\ -\frac{\partial \psi(R,t)}{\partial t} = (V(R) - E_T)\psi(R,t) \end{array} \right.$$

Trotter's theorem

- How do we find the solution of:

$$\frac{d\hat{\rho}}{dt} = (A + B)\hat{\rho}$$

- The operator solution is:

$$\hat{\rho} = e^{(A+B)t}$$

- Trotter's theorem (1959):

$$\hat{\rho} = \lim_{n \rightarrow \infty} \left[e^{\frac{t}{n}\hat{A}} e^{\frac{t}{n}\hat{B}} \right]^n$$

- Assumes that A,B and A+B are reasonable operators.

$$\left\langle R_0 \left| \left[e^{\frac{t}{n}\hat{A}} e^{\frac{t}{n}\hat{B}} \right]^n \right| R_n \right\rangle = \left\langle R_0 \left| e^{\frac{t}{n}\hat{A}} \right| R'_1 \right\rangle \left\langle R'_1 \left| e^{\frac{t}{n}\hat{B}} \right| R_1 \right\rangle \dots \left\langle R_{n-1} \left| e^{\frac{t}{n}\hat{A}} \right| R'_n \right\rangle \left\langle R'_n \left| e^{\frac{t}{n}\hat{B}} \right| R_n \right\rangle$$

- This means we just have to figure out what each operator does independently and then alternate their effect. This is rigorous in the limit as $n \rightarrow \infty$.
- In the DMC case A is diffusion operator, B is a branching operator.
- Just like “molecular dynamics” At small time we evaluate each operator separately.

Importance Sampling

Kalos 1970, Ceperley 1979

- Why should we sample the wavefunction? The physically correct pdf is $|\phi|^2$.
- Importance sample (multiply) by trial wavefunction.

$$f(R, t) \equiv \psi_T(R)\phi(R, t) \quad \lim_{t \rightarrow \infty} f(R, t) \equiv \psi_T(R)\phi_0(R)$$

$$-\frac{\partial f(R, t)}{\partial t} = \psi_T(R)H[f(R, t)/\psi_T(R)]$$

$$-\frac{\partial f(R, t)}{\partial t} = -\lambda \nabla^2 f - \lambda \nabla (2f \nabla \ln \psi_T(R)) + (\psi_T^{-1} H \psi_T) f(R, t)$$

- Evolution = diffusion + drift + branching
- Use accept/reject step for more accurate evolution.
make acceptance ratio > 99% . Determines time step.
- We have three terms in the evolution equation. Trotter's theorem still applies.

- To the pure diffusion algorithm we have added a drift step that pushes the random walk in directions of increasing trial function:

$$R' = R + 2\lambda\tau\nabla \ln \psi_T(R)$$

- Branching is now controlled by the local energy

$$E_L(R) - E_T = \psi^{-1}(R)\widehat{H}\psi(R) - E_T$$

- Because of zero variance principle, fluctuations are controlled.
- Cusp condition can limit infinities coming from singular potentials.
- We still determine E_T by keeping asymptotic population stable.

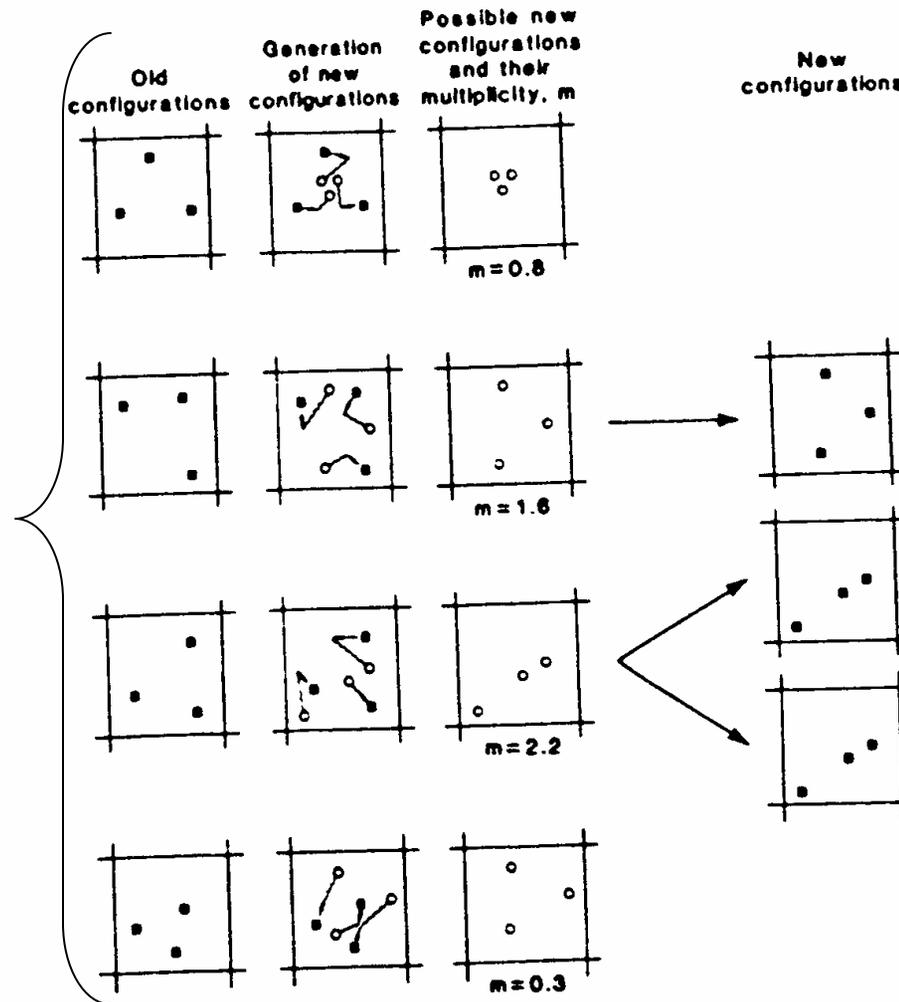
$$E_0 = \lim_{t \rightarrow \infty} \frac{\int dR \phi(R, t) H \psi_T(R)}{\int dR f(R, t)} \approx \left\langle E_\psi(R) \right\rangle_{f(\infty)}$$

Schematic of DMC

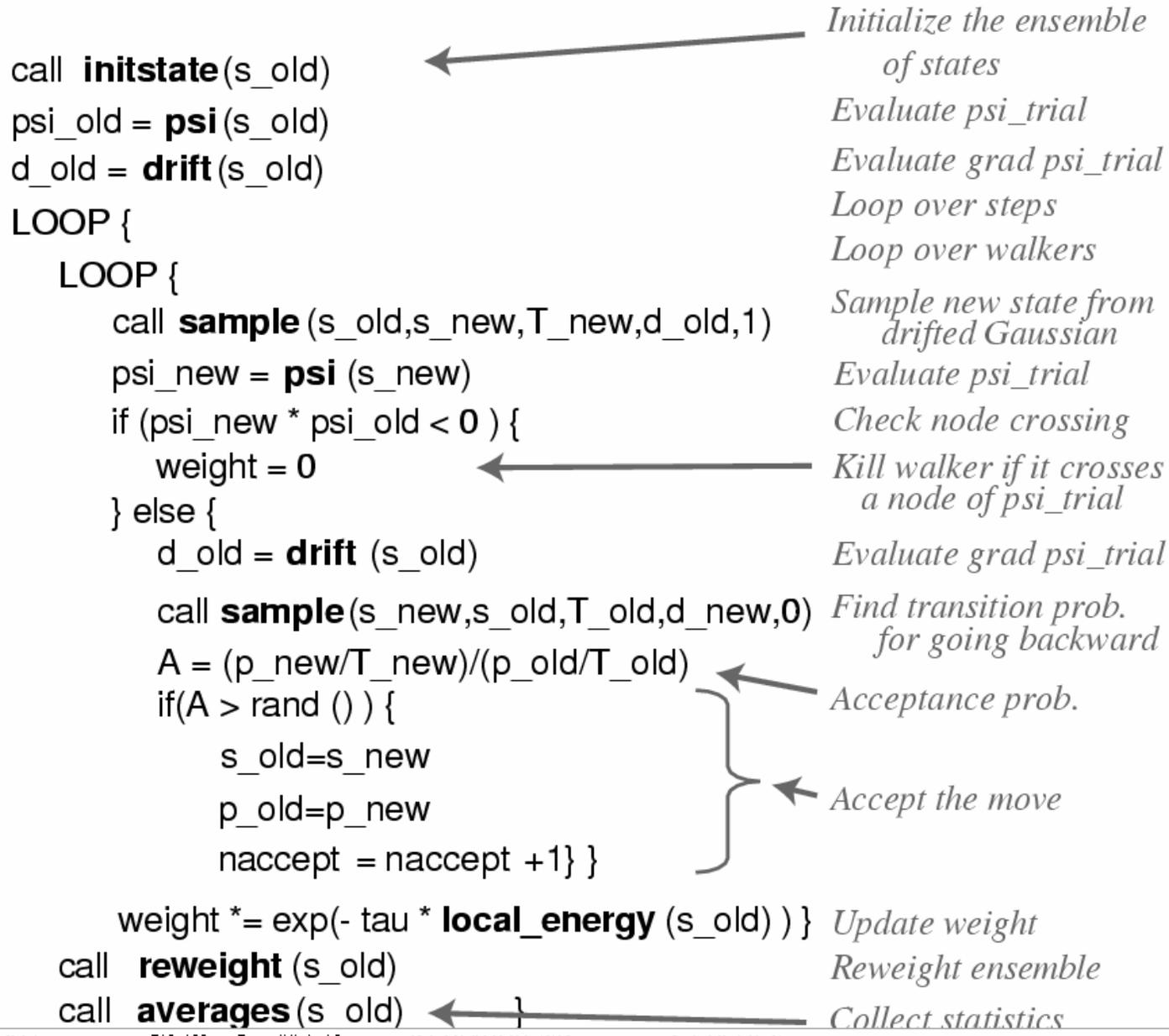
Ensemble evolves according to

- Diffusion
- Drift
- branching

ensemble



DIFFUSION MONTE CARLO CODE



Fixed-node method

- Initial distribution is a pdf.
It comes from a VMC simulation.
- Drift term pushes walks away from the nodes.
- Impose the condition:
- This is the fixed-node BC

$$f(R, 0) = |\psi_T(R)|^2$$

$$\phi(R) = 0 \quad \text{when} \quad \psi_T(R) = 0.$$

- Will give an upper bound to the exact energy, the best upper bound consistent with the FNBC.

$$E_{FN} \geq E_0$$

$$E_{FN} = E_0 \quad \text{if} \quad \phi_0(R)\psi(R) \geq 0 \quad \text{all } R$$

- $f(R,t)$ has a discontinuous gradient at the nodal location.
- Accurate method because Bose correlations are done exactly.
- Scales well, like the VMC method, as N^3 . Classical complexity.
- Can be generalized from the continuum to lattice finite temperature, magnetic fields, ...
- One needs trial functions with accurate nodes.

Fixed-Phase method

Ortiz, Martin, DMC 1993

- Generalize the FN method to complex trial functions: $\Psi(R) = e^{-U(R)}$
- Since the Hamiltonian is Hermitian, the variational energy is real:

$$E_V = \frac{\int dR e^{-2\Re U(R)} \left[V(R) + \lambda \nabla^2 U(R) - \lambda [\Re \nabla U(R)]^2 + \lambda [\Im \nabla U(R)]^2 \right]}{\int dR e^{-2\Re U(R)}}$$

- We see only one place where the energy depends on the phase of the wavefunction.
- If we **fix the phase**, then we add this term to the potential energy. In a magnetic field we get also the vector potential.

$$\text{effective potential} = V(R) + \sum_i \lambda_i \left[A(r_i) + \Im \nabla_i U(R) \right]^2$$

- We can now do VMC or DMC and get upper bounds as before.
- The imaginary part of the local energy will not be zero unless the right phase is used.
- Used for twisted boundary conditions, magnetic fields, vortices, phonons, spin states, ...

The mixed estimator problem

- Problem is that PMC samples the wrong distribution.

$$\langle A \rangle_M \equiv \frac{\int dR \psi^*(R) A \phi(R)}{\int dR \psi^*(R) \phi(R)}$$

- OK for the energy
- Linear extrapolation helps correct this systematic error

$$\langle A \rangle_o \equiv \frac{\int dR \phi^*(R) A \phi(R)}{\int dR \phi^*(R) \phi(R)}$$

$$\langle A \rangle_V \equiv \frac{\int dR \psi^*(R) A \psi(R)}{\int dR \psi^*(R) \psi(R)}$$

- Other solutions:

- Maximum overlap
- Forward walking
- Reptation/path integrals

$$\langle A \rangle_o \approx 2 \langle A \rangle_M - \langle A \rangle_V + O((\phi - \psi)^2)$$

$$\langle A \rangle_o \approx \frac{\langle A \rangle_M^2}{\langle A \rangle_V} + O((\phi - \psi)^2) \text{ for the density}$$

$$\langle A \rangle_M = \langle A \rangle_V \Rightarrow \int dR (\phi - \psi)^2 \text{ minimized wrt } A$$

Path Integral Monte Carlo

- We sample the distribution:

$$e^{-\sum_{i=1}^M S(\mathbf{R}_i, \mathbf{R}_{i+1}; \tau)} / Z \quad \text{where} \quad Z = \int d\mathbf{R}_1 \dots d\mathbf{R}_M e^{-\sum_{i=1}^M S(\mathbf{R}_i, \mathbf{R}_{i+1}; \tau)}$$

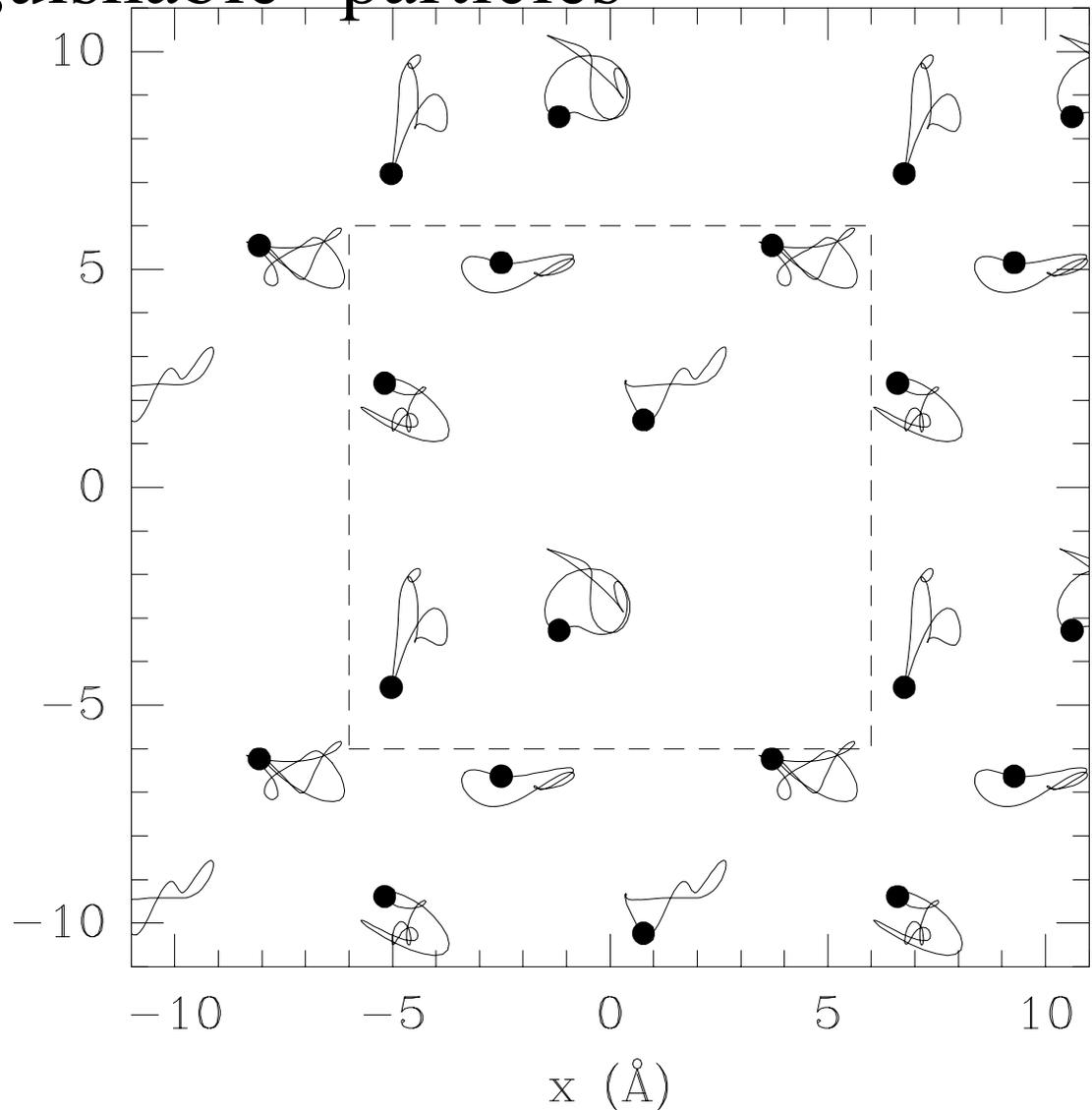
Where the “primitive” link action is:

$$S(\mathbf{R}_0, \mathbf{R}_1; \tau) = -\frac{3N}{2} \ln(4\pi\lambda\tau) + \frac{(\mathbf{R}_0 - \mathbf{R}_1)^2}{4\lambda\tau} + \frac{\tau}{2} [V(\mathbf{R}_0) + V(\mathbf{R}_1)]$$

- Similar to a classical integrand where each particle turns into a “polymer.”
 - K.E. is spring term holding polymer together.
 - P.E. is inter-polymer potential.
- Trace implies $\mathbf{R}_1 = \mathbf{R}_{m+1} \Leftrightarrow$ closed or ring polymers

“Distinguishable” particles

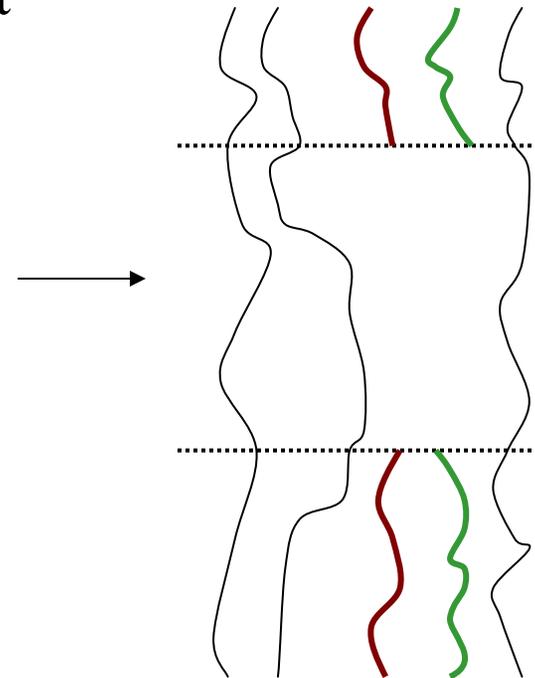
- Each atom is a ring polymer; an exact representation of a quantum wavepacket in imaginary time.
- Trace picture of 2D helium. The dots represent the “start” of the path. (but all points are equivalent)
- The lower the real temperature, the longer the “string” and the more spread out the wavepacket.



PIMC Sampling considerations

- Metropolis Monte Carlo that moves a single variable is too slow and will not generate permutations.
- We need to move many time slices together
- Key concept of sampling is how to sample a “bridge”: **construct a path starting at R_0 and ending at R_t .**
- How do we sample $R_{t/2}$? **GUIDING RULE.** Probability is:

$$P(R_{t/2}) = \frac{\langle R_0 | e^{-tH/2} | R_{t/2} \rangle \langle R_{t/2} | e^{-tH/2} | R_t \rangle}{\langle R_0 | e^{-tH} | R_t \rangle}$$



How to sample a single slice.

- pdf of the midpoint of the bridge:(a pdf because it is positive, and integrates to 1)
- For free particles this is easy-a Gaussian distribution

$$P(R_{t/2}) = \frac{\langle R_0 | e^{-tH/2} | R_{t/2} \rangle \langle R_{t/2} | e^{-tH/2} | R_t \rangle}{\langle R_0 | e^{-tH} | R_t \rangle}$$

PROVE: product of 2 Gaussians is a Gaussian.

$$R_{t/2} = \frac{1}{2}(R_0 + R_t) + \eta$$

$$\sigma^2 = \lambda t / 2 = \langle \eta^2 \rangle$$

- Interaction reduces P(R) in regions where spectator atoms are.
- Better is correlated sampling: we add a bias given by derivatives of the potential (for justification see RMP pg 326)
- Sampling potential U_s is a smoothed version of the pair action.

$$R_{t/2} = \frac{1}{2}(R_0 + R_t) + \lambda t \nabla U_s(R_{t/2}^0) + \eta$$

$$\overset{=2}{\sigma} = \lambda t / 2 \bar{I} + (\lambda t)^2 \bar{\nabla} \bar{\nabla} U_s(R_{t/2}^0) = \langle \bar{\eta} \bar{\eta} \rangle$$

$$U_s(R) = \text{sampling potential}$$

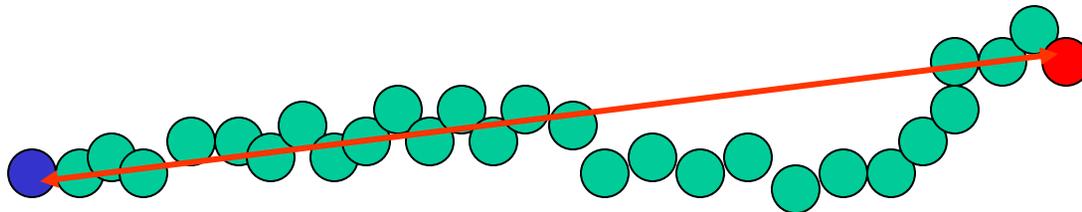
Reptation Monte Carlo (RQMC)

Ground State Path Integral (PIGS or GSPI)

- Similar technique to Diffusion MC:
 - Instead of (imaginary time=computer time), keep entire path in memory
 - Update with a Metropolis based method instead of branching diffusing random walks
- Two key questions:
 - How to move the paths?
 - Reptation means move like a snake. This is how polymers can move.
 - Bisection since they are path integrals
 - What to use for the action
 - DMC action
 - Path Integral action
- Advantages
 - Get exact properties: no forward walking or mixed estimators
 - Good for energy differences.

Polymer Reptation (slithering snake)

- Polymers move very slowly because of entanglement.
- A good algorithm is "reptation."
 - *Choose end at random.*
 - *Cut off one end and stick onto the other end.*



- Sample directly the bonding interaction
- Acceptance probability is change in non-bonding potential.
- Simple moves go quickly through polymer space.
 - But Ergodic? Not always (what if both ends get trapped?)
- Decorrelation time is $O(N^2)$..
- Completely unphysical dynamics or is it?
 - This is how entangled polymers actually move. (theory of de Gennes)

Ground State Path Integrals

Project a trial function as in DMC.

$$\Psi(\beta) = e^{-\frac{\beta}{2}H} \Psi$$

$\psi(\beta)$ converges to the exact ground state as a function of imaginary time.

$$E(\beta) = \frac{\langle \Psi(\beta) H \Psi(\beta) \rangle}{\langle \Psi(\beta) \Psi(\beta) \rangle} = \langle E_L(R_0) \rangle_\beta$$

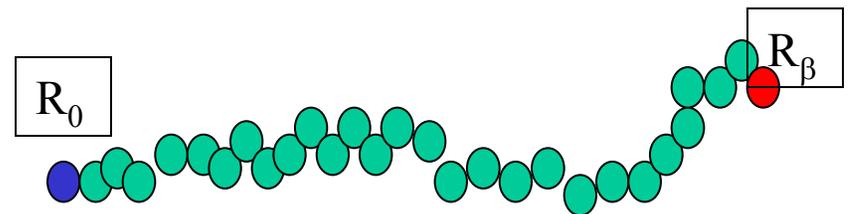
$E(\beta)$ is an upper bound converging to the exact answer monotonically

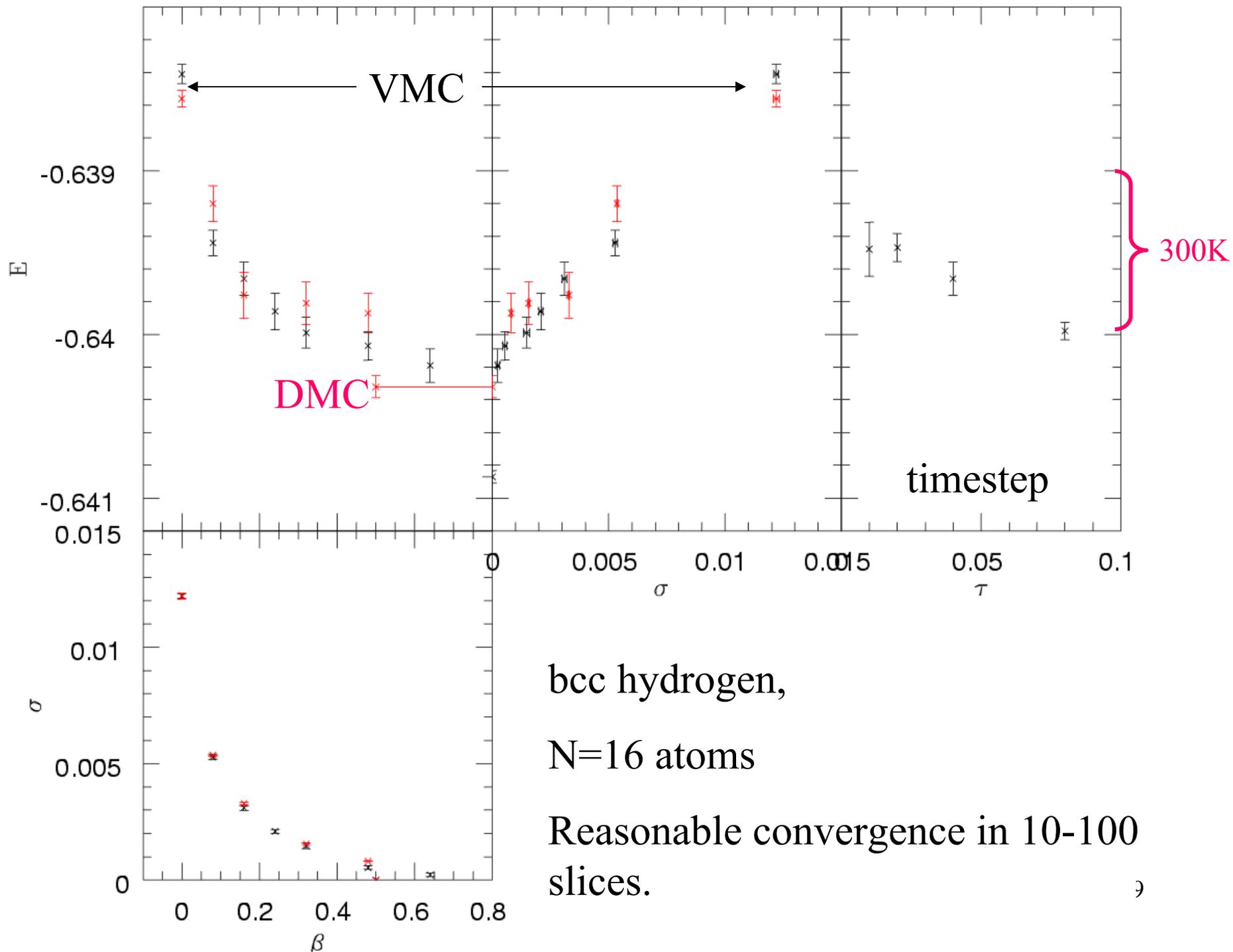
$$Z(\beta) = \langle \Psi(\beta) \Psi(\beta) \rangle = \langle \Psi e^{-\beta H} \Psi \rangle = \int dR_0 \dots dR_p \Psi(R_0) \langle R_0 e^{-\tau H} R_1 \rangle \dots \langle R_{p-1} e^{-\tau H} R_p \rangle \Psi(R_p)$$

$$\tau = \frac{\beta}{p} = \text{timestep}$$

Do Trotter break-up into a path of p steps

$$\sigma^2(\beta) = \langle \delta E_L(R_0) \delta E_L(R_p) \rangle = -\frac{dE(\beta)}{d\beta}$$





Metropolis algorithm

Three key concepts:

1. Sample by using an ergodic random walk.
2. Determine equilibrium state by using detailed balance
3. Achieve detailed balance by using rejections.

Detailed balance: $\pi(s) P(s \rightarrow s') = \pi(s') P(s' \rightarrow s)$.

Rate balance from s to s' .

Put $\pi(s)$ into the master equation.

$$\sum_s \pi(s) P(s \rightarrow s') = \sum_s \pi(s') P(s' \rightarrow s) = \pi(s') \sum_s P(s' \rightarrow s) = \pi(s')$$

- Hence $\pi(s)$ is an eigenfunction.
- If $P(s \Rightarrow s')$ is ergodic then $\pi(s)$ is the unique steady state solution.

General Metropolis MC

Metropolis achieves detailed balance by *rejecting* moves.
Break up transition probability into sampling and acceptance:

$$P(s \rightarrow s') = T(s \rightarrow s') A(s \rightarrow s')$$

$$T(s \rightarrow s') = \text{sampling probability}$$

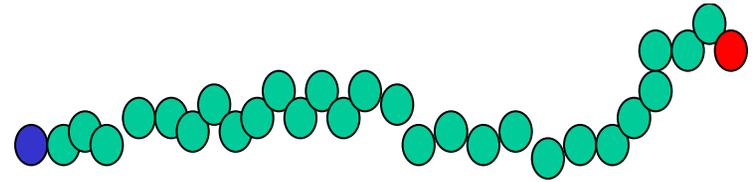
$$A(s \rightarrow s') = \text{acceptance probability}$$

The optimal acceptance probability that gives detailed balance is:

$$A(s \rightarrow s') = \min \left[1, \frac{T(s' \rightarrow s)\pi(s')}{T(s \rightarrow s')\pi(s)} \right]$$

Note that normalization of $\pi(s)$ is not needed or used!

Reptation moves



- Let d be the direction of the move

-1 tail move

+1 head move

$$T_d (s \rightarrow s')$$

- Standard method.

- Choose “ d ” at random:

- Acceptance probability is:

$$T(s \rightarrow s') = \frac{1}{2} [T_{-1}(s \rightarrow s') + T_1(s \rightarrow s')] \quad a = \frac{T(s' \rightarrow s)\pi(s')}{T(s \rightarrow s')\pi(s)} = \frac{T_{-d}(s' \rightarrow s)\pi(s')}{T_d(s \rightarrow s')\pi(s)}$$

- Sample the same Gaussian used in DMC!

- Change in action involves wavefunction at new point, and previously saved numbers Takes $O(p^2)$ steps to decorrelate..

- One way reptation gives the wrong answers.

- Bounce method:

- add “ d ” to the state.

- Change “ d ” only on rejections.

- Use same acceptance formula!!

- Does not satisfy detailed balance but still gives correct answer since it is an eigenfunction of T .

- Moves are $1/(\text{rejection rate})$ times more effective!

Link action

- PIMC method: pair action plus nodal action
- DMC method. Use importance-sampled evolution to suggest action (good for accurate trial functions)

$$\langle R | e^{-\tau H} | R' \rangle = \frac{\psi(R')}{\psi(R)} \exp \left[-\frac{(R' - R - \tau F)^2}{4\lambda\tau} - \tau E_L(R) \right]$$

Symmetrize with respect to R and R' to get higher accuracy.

- time step is longer in RQMC than in DMC because action is symmetric (Hermitian).
 - For fixed-phase: add a potential to avoid the sign problem. Exact answer if potential is correct.
- $$\boxed{(\text{Im } \nabla \ln \Psi)^2}$$
- Local energy enters through the acceptance rate and not through the branching.

Averages

- Take them in the middle of the reptile.

$$\langle O \rangle = \lim_{\beta \rightarrow \infty} \langle \Psi(\beta) O \Psi(\beta) \rangle = \langle O(R_{p/2}) \rangle$$

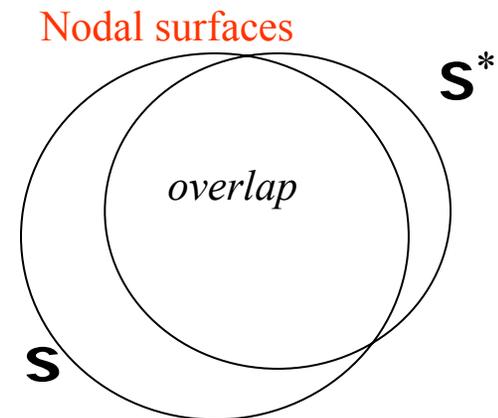
- But you need to make p twice as large for averages (energy always converges faster)
- Forward walking with DMC is inherently unstable for long projection times because of weight fluctuations.
- No instability in RQMC; perhaps an ergodic problem.
- Little loss of efficiency in taking the middle with bounce algorithm, since every point is the middle one time.

Energy difference methods

- We need a fast way of computing difference:
[E(S)-E(S*)]
- Naïve (direct) method is to do separate (uncorrelated) samples of S and S*. Noise increases by $\sqrt{2}$.
- Correlated methods map S walks into S* walks.
- Simplest is “VMC re-weighting” (1-sided)
- With fixed-node fermions, we need to worry about changes in the nodal surfaces. 1-sided methods can give the wrong answer because the distributions are not defined in the same regions of path space.
- Reptation is convenient because we know the probability for a path.

$$E(S^*) \approx \frac{\sum_{i=1}^M w_i(S^*) E_L(R_i; S^*)}{\sum_{i=1}^M w_i(S^*)}$$

$$w_i(S^*) = \frac{|\psi_T(R_i; S^*)|^2}{P(R_i)}$$



“Reptile” space

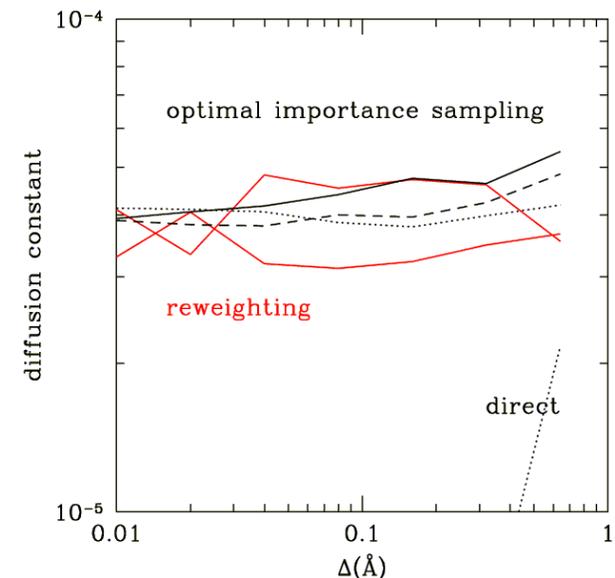
Optimal Importance Sampling

- What distribution has the lowest variance for the energy difference? (ignoring autocorrelation effects)

$$\rho(s) \propto \left| \Psi_1(s)^2 \Delta E_{L1} - \Psi_2(s)^2 \Delta E_{L2} \right|$$

$$\rho(s) \sim \left| \Psi_1(s) \right|^2 + \left| \Psi_2(s) \right|^2$$

- Sum of squares is almost as good, and eliminates barriers which might be hard to cross.
- Symmetric in the two distributions.
- 2 orders of magnitude faster



COMPARISON OF METHODS

they are all based on thermal density matrix

they share features: the action, the sampling

DMC

- State space: P walkers
- Action/Dynamics determined by H
- Observables have mixed estimator problem-need to do forward walking
- No permutations
- Trial function & trial energy
- Population bias
- Energy is “zero variance”

$$\langle R | e^{-\tau H} | R' \rangle$$

PIMC

- State space: closed path & permutation
- Action fixed/Dynamics arbitrary
- Observables anywhere
- Particle statistics=Permutations
- Temperature>0! T=0 expensive.

RQMC

- State space: reptile & direction
- Action fixed/Dynamics arbitrary
- Single particle moves more difficult
- Observables from middle of path
- Trial function
- Projection bias
- Energy is “zero variance”

Calculation of excited-state energies

Correlation Function MC: J. Chem. Phys. **89**, 6316 (1988).

- No fixed-node upper bound for all excited states.
- Construct a basis of trial functions spanning excited states in question. $\{f_i(R)\} \quad 1 \leq i \leq M$
- Using VMC, calculate all the matrix elements as a function of imaginary time

- Find lowest energy in this basis
- Solve the generalized eigenvalue problem:

- McDonald's theorem

$$H_{ij}(t)C_i^\lambda = E(t)^\lambda N_{ij}(t)C_i^\lambda$$

$$N_{ij}(t) \equiv \langle f_i | f_j \rangle$$

$$H_{ij}(t) \equiv \langle f_i | H | f_j \rangle$$

- Then E_k approaches the exact eigenvalue from above.
- Use correlated sampling to calculate all energies together.

Best guiding function:

$$|\psi|^2 = \sum_n |f_n|^2$$

Properties of solution to GEP

- For a basis of size m , there exist “ m ” eigenvalues and orthonormal eigenfunctions:

$$\psi_n(R) = \sum_{k=1}^m a_{k,n} f_k(R)$$

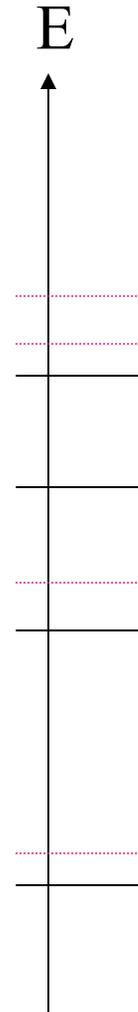
$$\langle \psi_n | \psi_m \rangle = a_n^* S_{nm} a_m = \delta_{nm}$$

- McDonald’s theorem: the n^{th} eigenvalue in a basis is an upper bound to the n^{th} “exact eigenvalue.

$$E_0 \leq E_1 \leq E_2 \leq \dots \leq E_m$$

$$E_n^{ex} \leq E_n$$

- We can always lower all the energies by augmenting the basis
- When basis is complete, we get exact answers!
- Orthogonality taken into account in the solution.



Diffusion/Reptation Monte Carlo method

- The time-evolved basis approaches the exact eigenfunctions:

$$f_i(R, t) = e^{-tH/2} f_i(R)$$

- Using bosonic DMC (no nodes) or reptation calculate the N and H as a function of imaginary time. Note, $H=dN/dt$.

$$N_{ij}(t) \equiv \left\langle f_i \left| e^{-t\hat{H}} \right| f_j \right\rangle$$

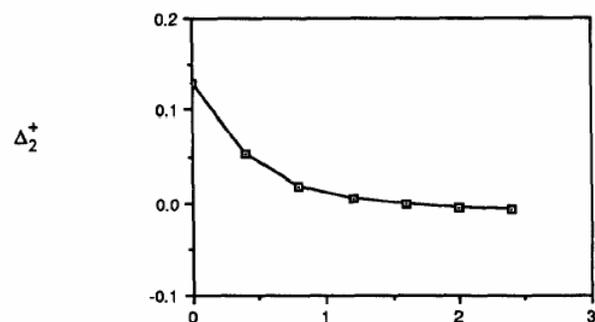
- In reptation it is the end-end correlation function
- Use same guiding function for importance sampling.
- Solve the generalized eigenvalue problem:

$$H_{ij}(t) a_i^\lambda = E(t)^\lambda N_{ij}(t) a_i^\lambda$$

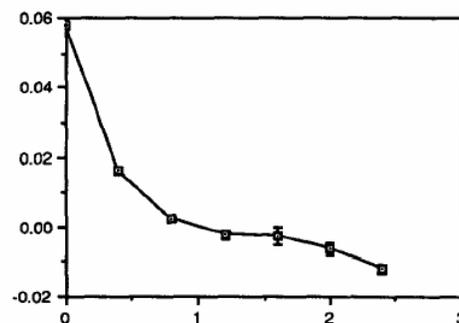
- Then $E^\lambda(t)$ approaches the exact λ^{th} energy exponentially fast and from above.

Typical results

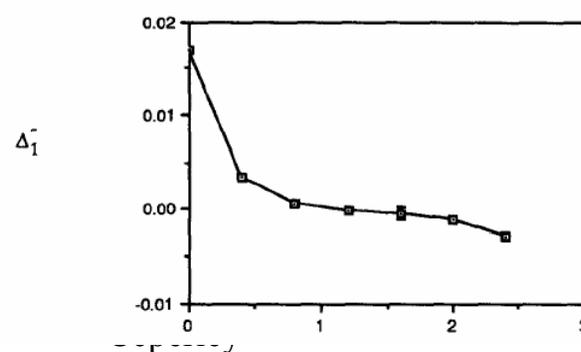
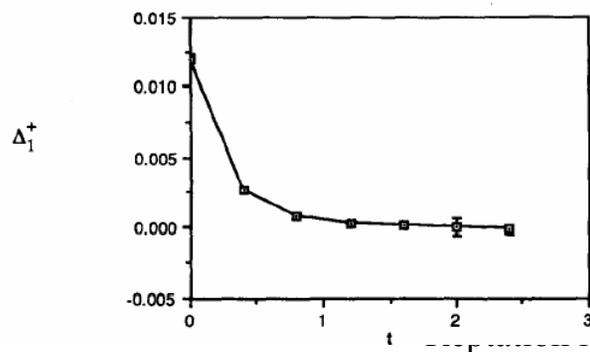
- Look for plateau in energy.
- Error bars grows exponentially in time (sign problem).
- Best results are for lower energy states
- Can use symmetry to reduce matrix size.



(b)



(e)



Remarks on CFMC

- Zero variance principle applies.
- Can treat a large basis and hence get a whole spectrum at once.
- Sign problem is still there. In practice “ t ” cannot be too large.
- If nodes in the DMC are present, excited state energies will be wrong.
- Maybe MaxEnt methods can do better. But problems working in energy space. Much better in effective Hamiltonian space.
- Difficult to make realistic basis for many-body systems.

Exciton-Exciton scattering

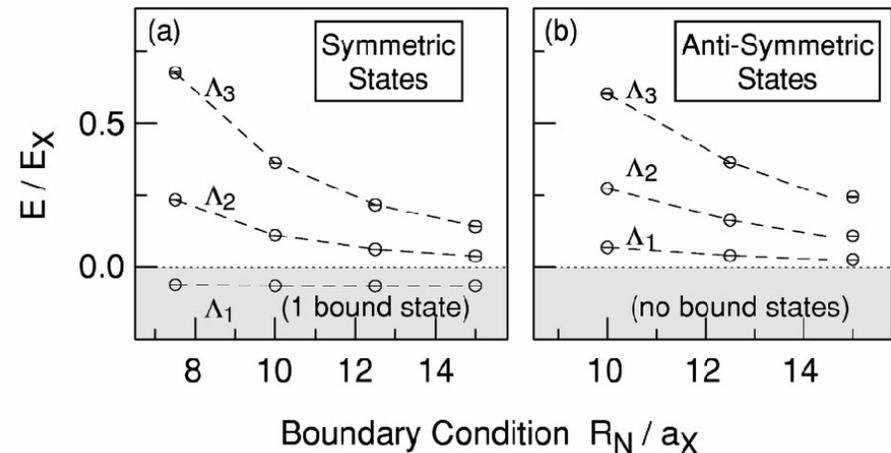
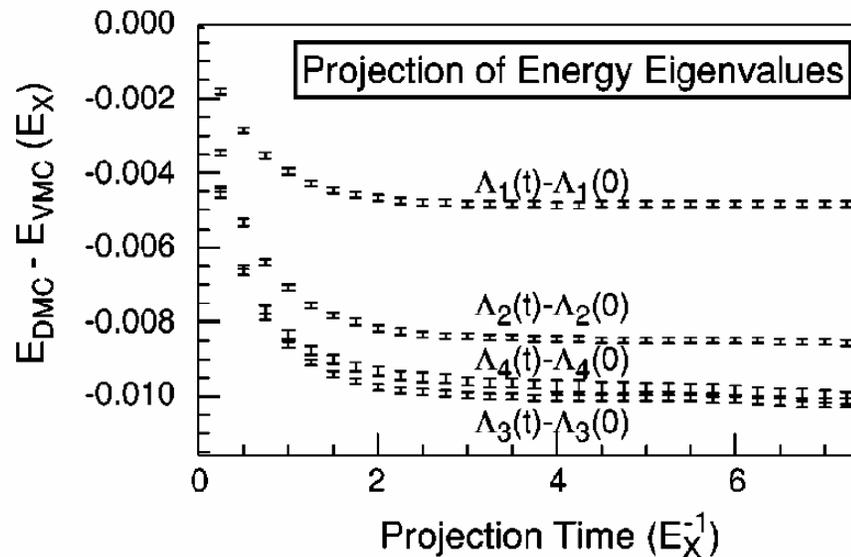
Shumway and DC, *Phys. Rev. B* 63, 165209-165215 (2001).

- 4-quantum particles
- Boundary conditions and energy determine phase shifts
- Use excited state method to get exact energies inside boundaries.



$$r_c \Rightarrow E_0, E_1, E_2, \dots \Rightarrow k_0, k_1, k_2, \dots$$

$$(r_c, k_n) \Rightarrow \delta(k_n) \Rightarrow \sigma(k)$$



Imaginary time correlations

- With PIMC and DMC we can calculate imaginary time dynamics:

$$F_O(\tau) = Z^{-1} \left\langle O e^{-\tau \hat{H}} O e^{-(\beta-\tau) \hat{H}} \right\rangle$$

(DMC corresponds to $\beta \rightarrow \infty$)

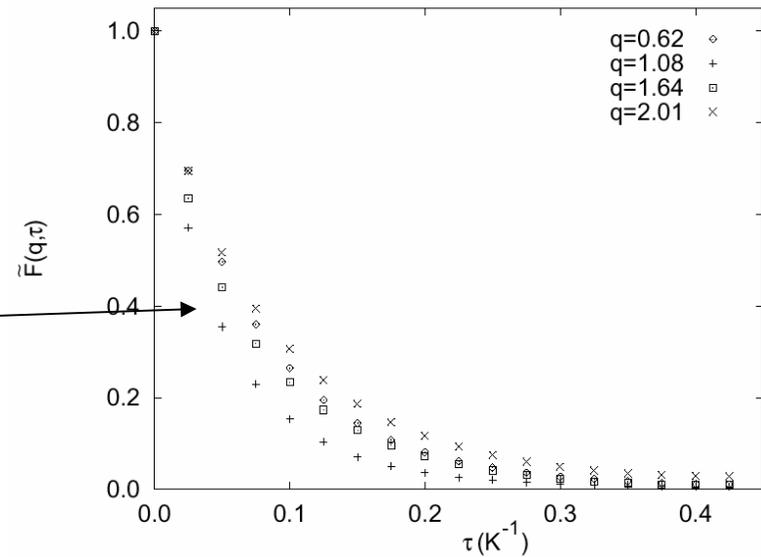
- If we could determine this analytically we could just substitute imaginary values of τ for real values.
- Dynamic structure function is the response to a density perturbation is (e.g. density-density response)

$$S_k(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i\omega t} F_k(t) \quad \text{where } O = \frac{1}{\sqrt{N}} \sum_{i=1}^N e^{i\vec{k} \cdot \vec{r}_i}$$

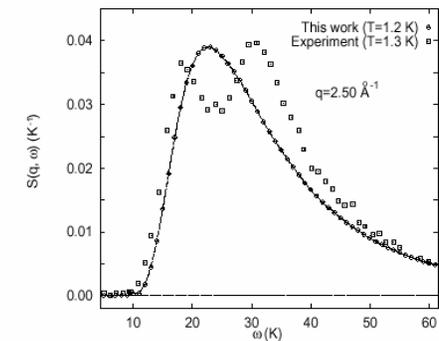
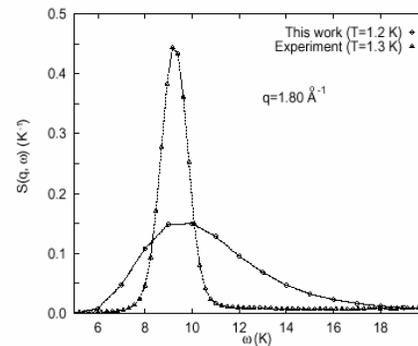
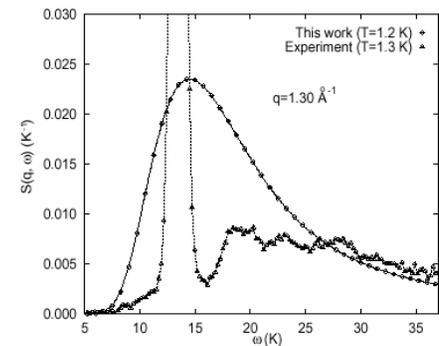
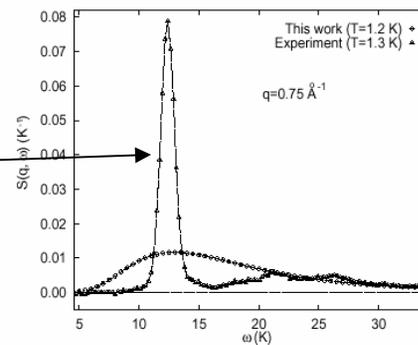
$$F_k(\tau) = \int_{-\infty}^{\infty} d\omega e^{-\tau\omega} S_k(\omega)$$

$$F_o(\tau) = Z^{-1} \left\langle O e^{-\tau \hat{H}} O e^{-(\beta-\tau) \hat{H}} \right\rangle$$

Little structure or information in $F(q,t)$



but much in $S(k,w)$.
Sharp peaks at the excitations.



Bayes' theorem

- What is the most probable value of $S_k(\omega)$ given:
 - The PIMC data
 - Prior knowledge of $S_k(\omega)$.
- Bayes' theorem (also used by Laplace)

$$\Pr(S(\omega)|F(t)) \propto P_L(F(t)|S(\omega)) P_p(S(\omega))$$

- Likelihood function follows from central limit theorem:

$$P_L(F(t)|S(\omega)) \propto \exp\left[-\frac{1}{2} \sum_{\tau, \tau'} \delta F(\tau) \sigma(\tau, \tau')^{-1} \delta F(\tau')\right]$$

$$\delta F(\tau) = F(\tau) - \langle F(\tau) \rangle \quad \text{and} \quad \sigma(\tau, \tau') = \langle \delta F(\tau) \delta F(\tau') \rangle$$
- But what to choose for the prior $P_p(S)$? Typical choice is the “entropy.”

$$P_p(S(\omega)) \propto \exp\left[\alpha \sum_{\omega} S(\omega) \ln(S(\omega) / m(\omega))\right]$$

Now two routes to making the inversion:

1. Sample $S_k(w)$. **AvEnt** Using MCMC make moves in $S_k(w)$ space. Take averages and also get idea of the allowed fluctuations. Model defined self consistently
2. Find most probable $S_k(w)$. **MaxEnt** Maximize function. Ok if the p.d.f. is highly peaked. Estimate errors by the curvature at the maximum. Fast to do numerically but makes more assumptions.

How do we choose α ? Choose it from its own prior function so the strength of the likelihood function and the prior function are balanced.

$$P(\alpha) = 1/\alpha.$$

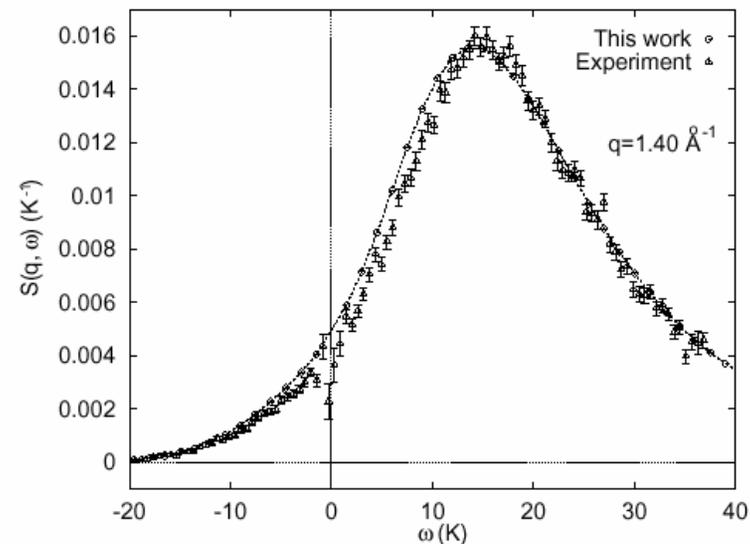
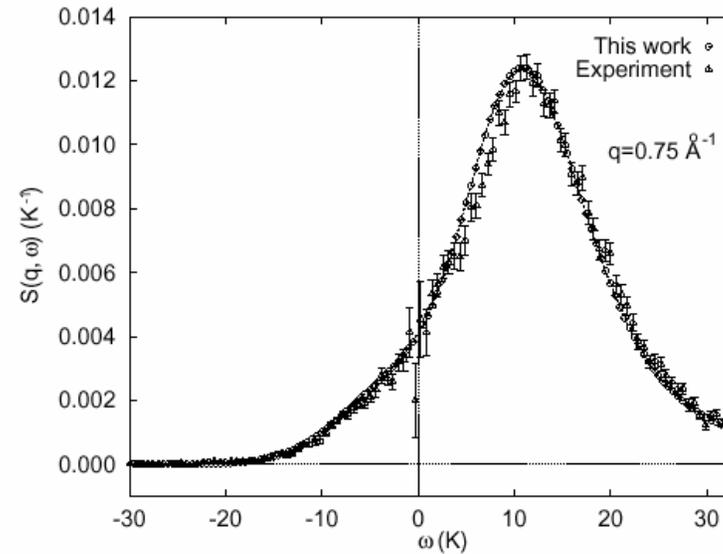
Example: Liquid ^4He

Boninsegni and DMC

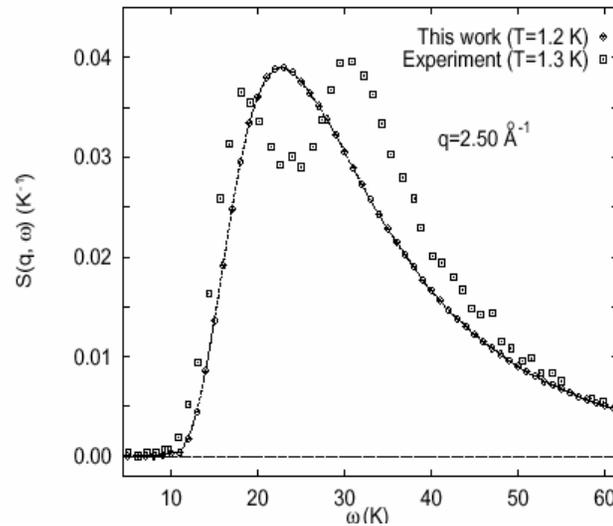
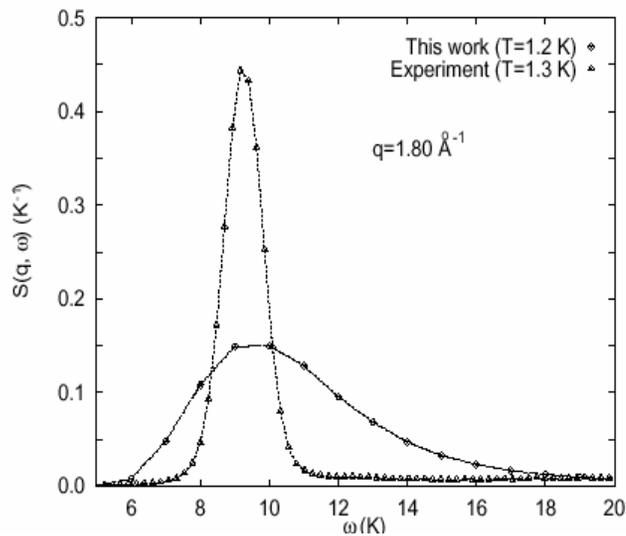
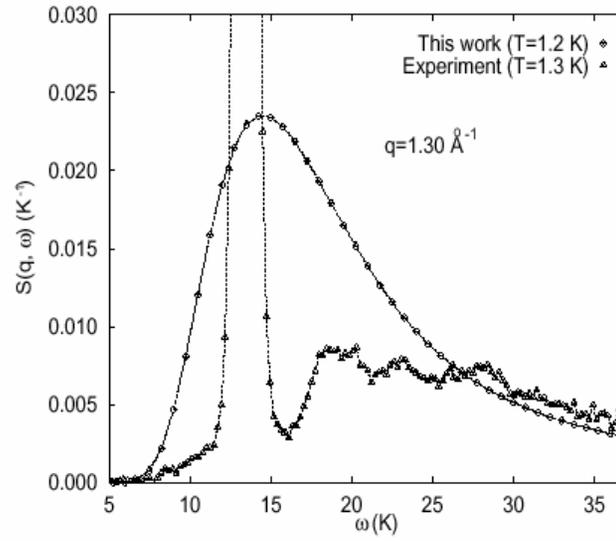
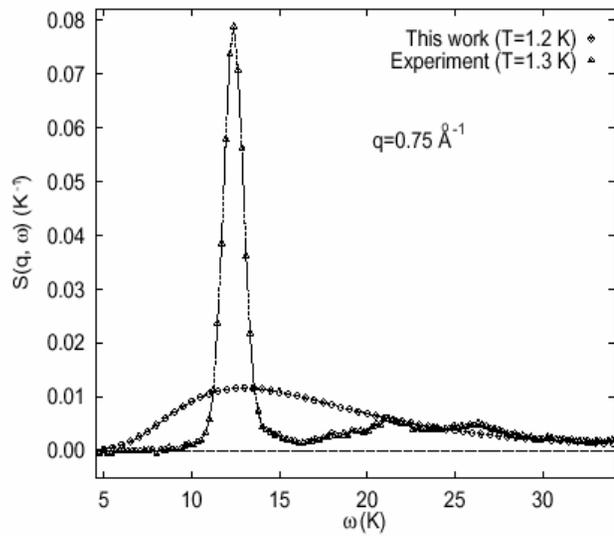
- Calculate $F_k(\tau)$ using PIMC (UPI).
- AvEnt works beautifully in normal phase.
- Gives peaks too broad in the superfluid phase. **Failure of the entropic prior.**
- It makes the assumption that energy modes are uncoupled. This is false! Energy levels repel each other so that if there is energy at one level, it is unlikely at nearby values.
- Would require incredible precision to get sharp features.
- But good method for determining the excitation energy.

Comparison in normal liquid He phase

- MaxEnt works well in normal phase ($T=4\text{K}$)
- Modes are quantum but independent of each other



Comparison in Superfluid



Excitation energies

- Better PIMC data, more time values, smaller errors.
- Better to work in effective hamiltonian space, not energy space.
- Get more information, for example,
 - multiphonon correlation functions
 - Incorporate exchange values
 - Analytic information about response properties

Reasonable excitation energies

